

Supplementary Information

Effect of N-1 arylation of monastrol on kinesin Eg5 inhibition in Glioma cell lines.

Itamar Luís Gonçalves^{1¥}, Liliana Rockenbach^{1¥}, Gustavo Machado das Neves¹, Gabriela Göethel², Fabiana Nascimento¹, Luciano Porto Kagami¹, Fabrício Figueiró³, Gabriel Oliveira de Azambuja¹, Amanda de Fraga Dias³, Andressa Amaro³, Lauro Mera de Souza⁴, Ivan da Rocha Pitta⁵, Daiana Silva Avila⁶, Daniel Fábio Kawano⁷, Solange Cristina Garcia², Ana Maria Oliveira Battastini³, Vera Lucia Eifler-Lima*¹.

¹Laboratório de Síntese Orgânica Medicinal/LaSOM, Faculdade de Farmácia, Universidade Federal do Rio Grande do Sul. Avenida Ipiranga, 2752, Porto Alegre / RS, Brazil.

² Laboratório de Toxicologia –LATOX, Faculdade de Farmácia, Universidade Federal do Rio Grande do Sul, Porto Alegre/RS, Brazil.

³Departamento de Bioquímica, ICBS, Universidade Federal do Rio Grande do Sul, Porto Alegre/RS, Brazil

⁴ Instituto de Pesquisa Pelé Pequeno Príncipe, Faculdades Pequeno Príncipe, Curitiba-PR, Brazil

⁵UFPE

⁶ Grupo de Pesquisa em Bioquímica e Toxicologia em Caenorhabditis elegans (GBToxCE), Universidade Federal do Pampa-UNIPAMPA, BR 592, Km 472, CEP 97500-970 Uruguaiana, RS, Brazil

⁷ Faculdade de Ciências Farmacêuticas, Universidade Estadual de Campinas, Campinas-SP, Brazil

¥ Author Contributions: These authors contributed equally to this work.

* Corresponding authors: veraeifler@ufrgs.br

Table of contents

Figure S1. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 19a	3
Figure S2. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19a	4
Figure S3. HRMS spectrum of compound 19a	5
Figure S4. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 20a	6
Figure S5. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 20a	7
Figure S6. HRMS spectrum of compound 20a	8
Figure S7. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 19b	9
Figure S8. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19b	10
Figure S9. HRMS spectrum of compound 19b	11
Figure S10. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 20b	12
Figure S11. ^{13}C NMR spectrum (15 MHz, $\text{DMSO}-d_6$) of compound 20b	13
Figure S12. HRMS spectrum of compound 20b	14
Figure S13. ^1H NMR spectrum (60 MHz, $\text{DMSO}-d_6$) of compound 19e	15
Figure S14. ^{13}C NMR spectrum (15 MHz, $\text{DMSO}-d_6$) of compound 19e	16
Figure S15. HRMS spectrum of compound 19e	17
Figure S16. ^1H NMR spectrum (60 MHz, $\text{DMSO}-d_6$) of compound 20e	18
Figure S17. ^{13}C NMR spectrum (15 MHz, $\text{DMSO}-d_6$) of compound 20e	19
Figure S18. HRMS spectrum of compound 20e	20
Figure S19. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 19h	21
Figure S20. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19h	22
Figure S21. HRMS spectrum of compound 19h	23
Figure S22. ^1H NMR spectrum (60 MHz, $\text{DMSO}-d_6$) of compound 20h	24
Figure S23. ^{13}C NMR spectrum (15 MHz, $\text{DMSO}-d_6$) of compound 20h	25
Figure S24. HRMS spectrum of compound 20h	26
Figure S25. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 19k	27
Figure S26. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19k	28
Figure S27. HRMS spectrum of compound 19k	29
Figure S28. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 20k	30
Figure S29. ^{13}C NMR spectrum (15 MHz, $\text{DMSO}-d_6$) of compound 20k	31
Figure S30. HRMS spectrum of compound 20k	32

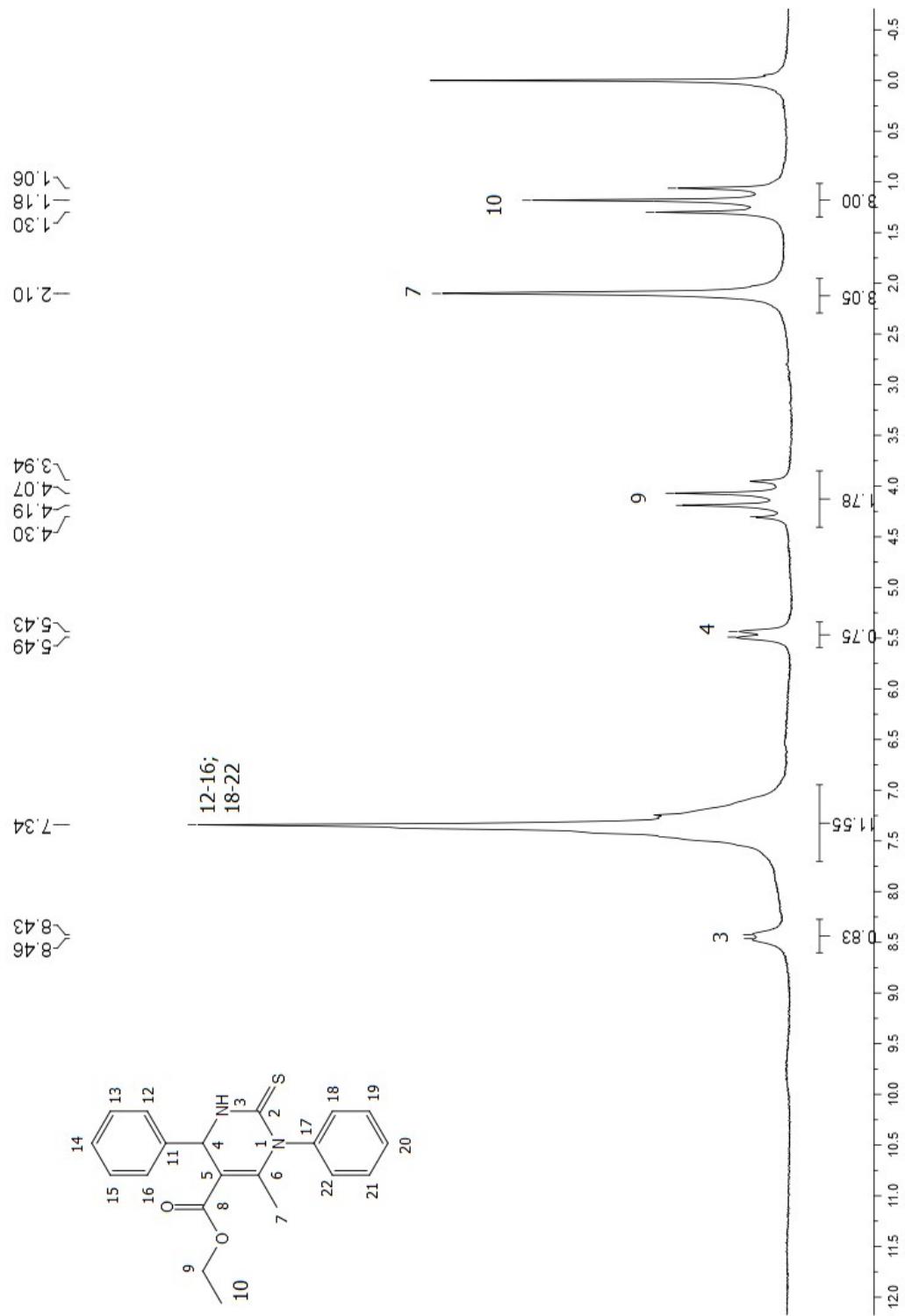


Figure S1. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 19a.

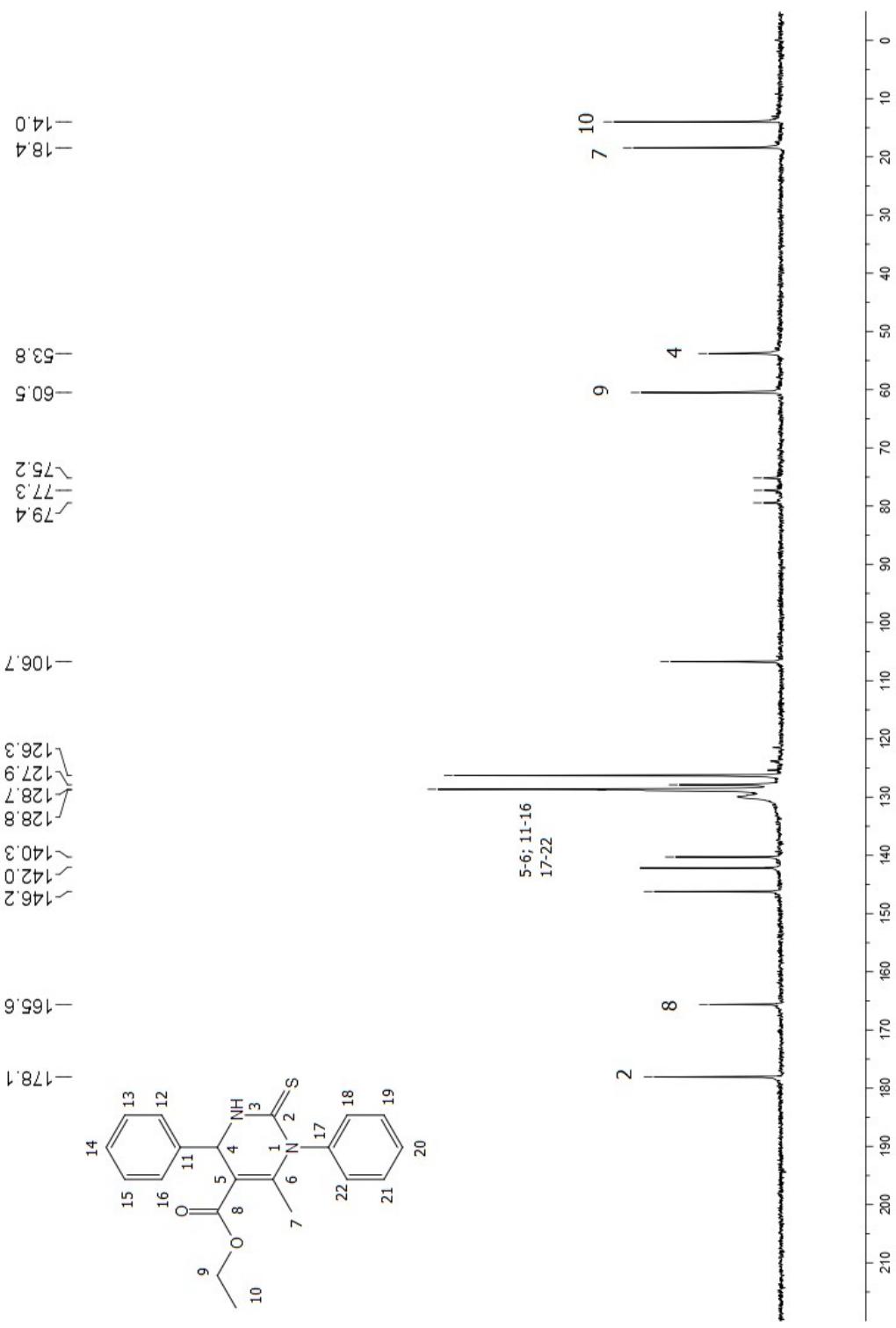


Figure S2. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19a.

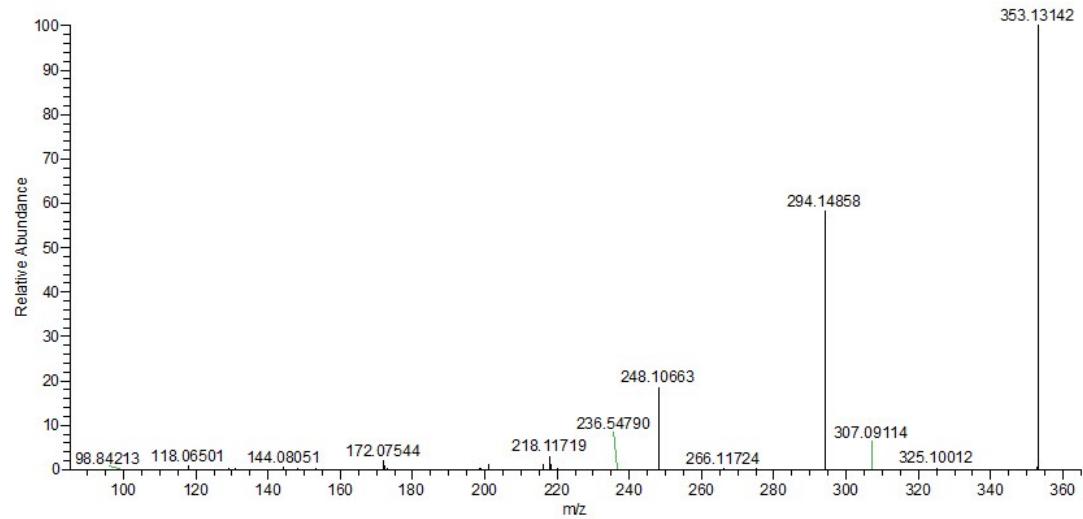
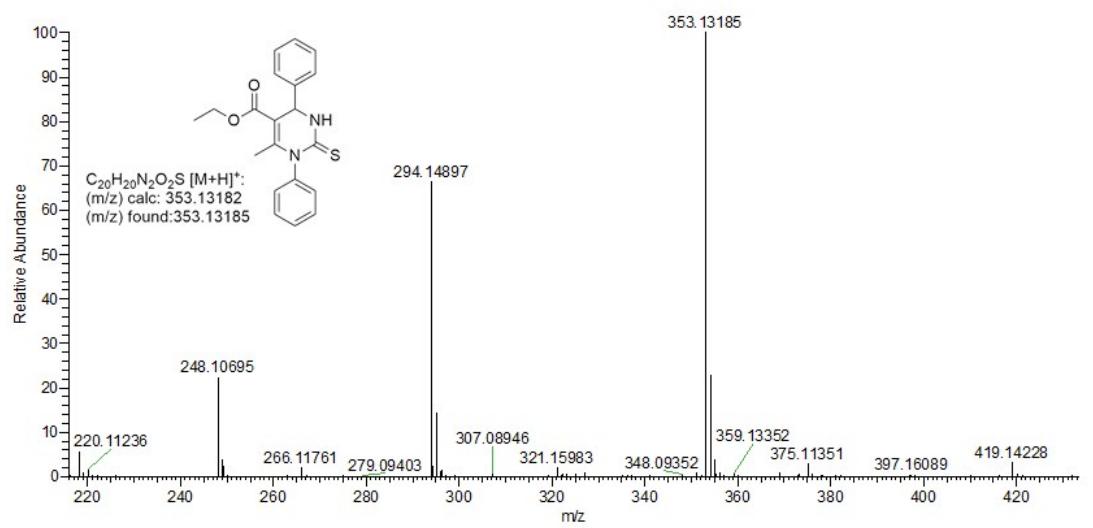


Figure S3. HRMS spectrum of compound 19a.

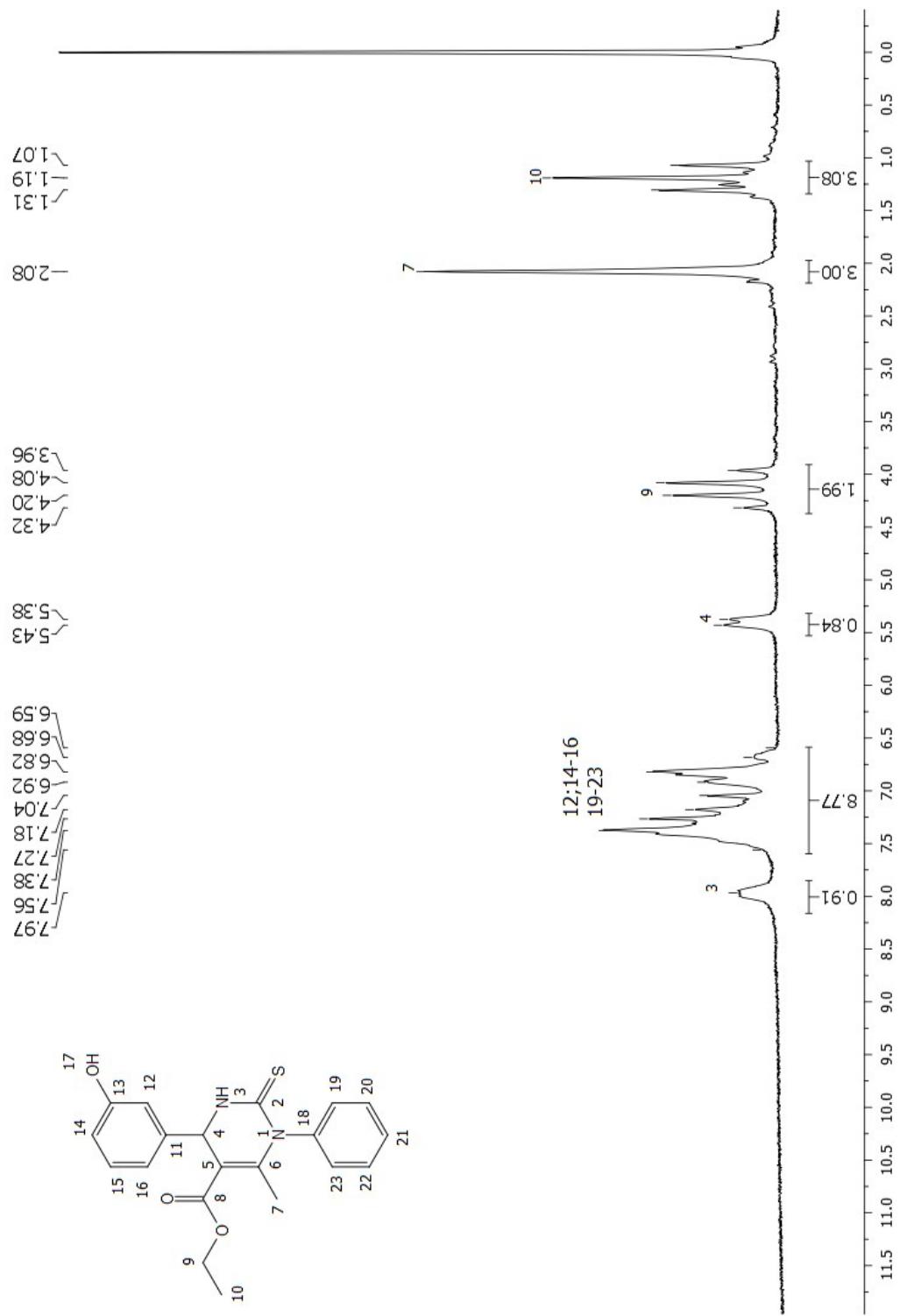


Figure S4. ¹H NMR spectrum (60 MHz, CDCl₃) of compound 20a.

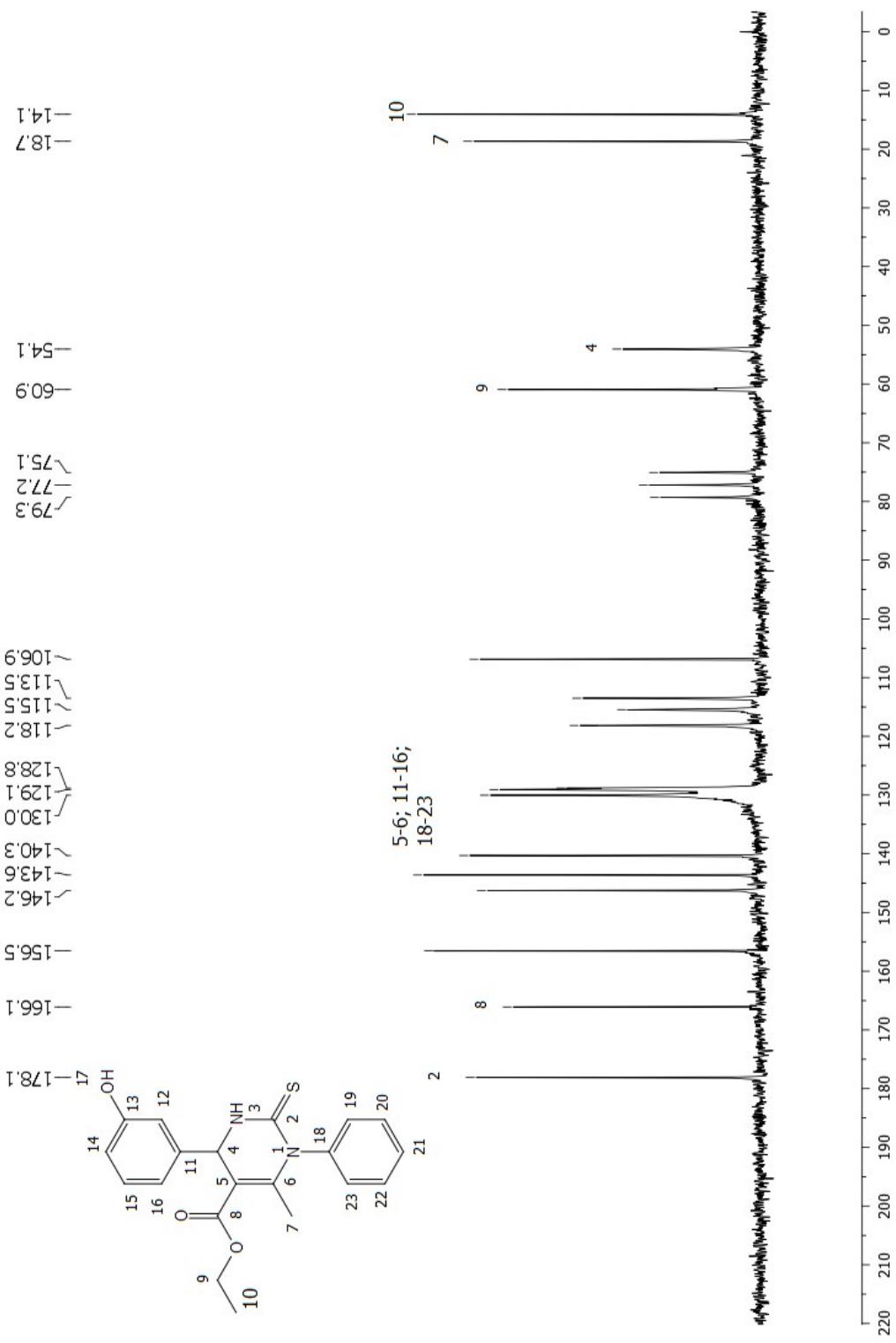


Figure S5. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 20a.

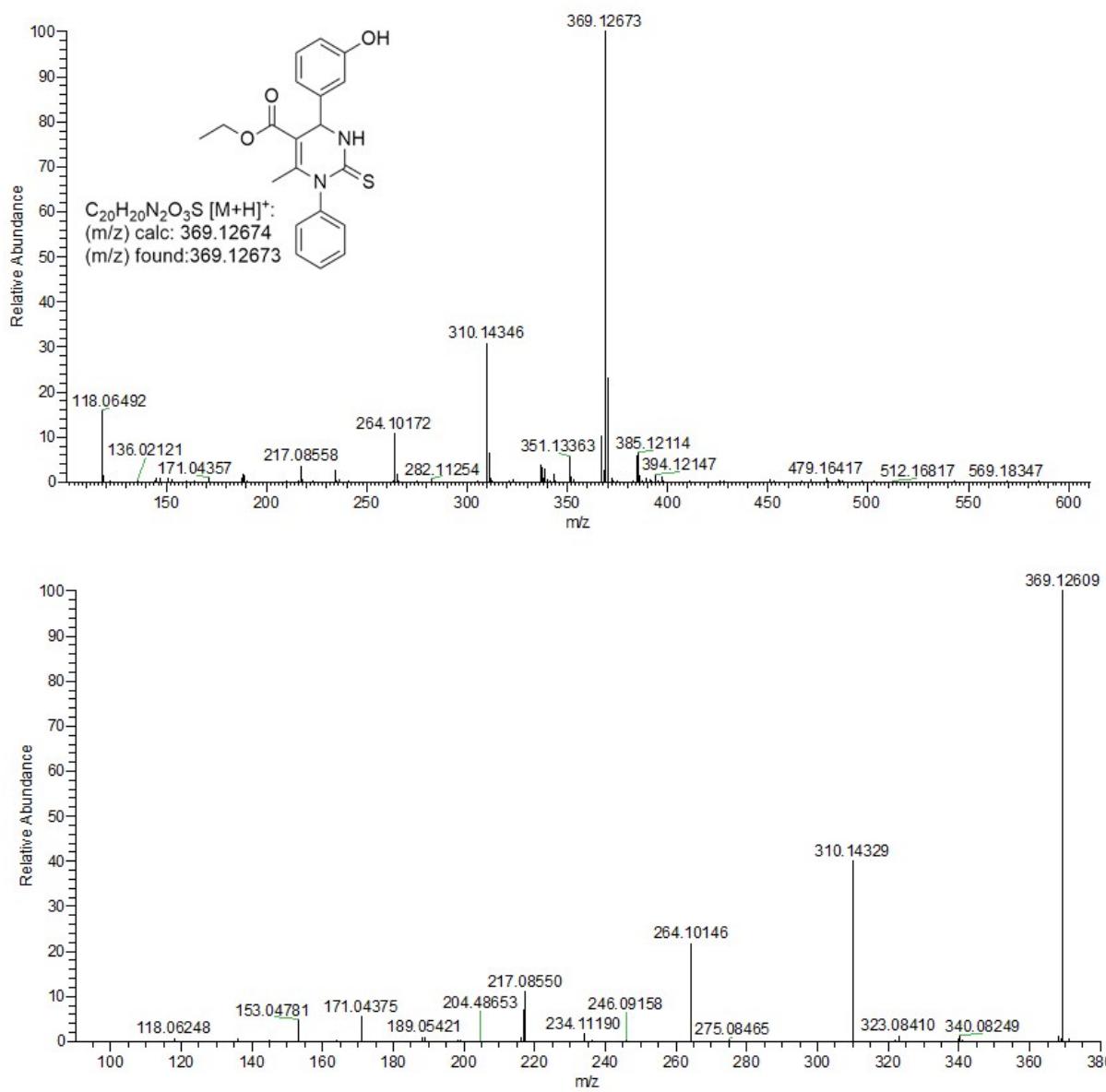


Figure S6. HRMS spectrum of compound **20a**.

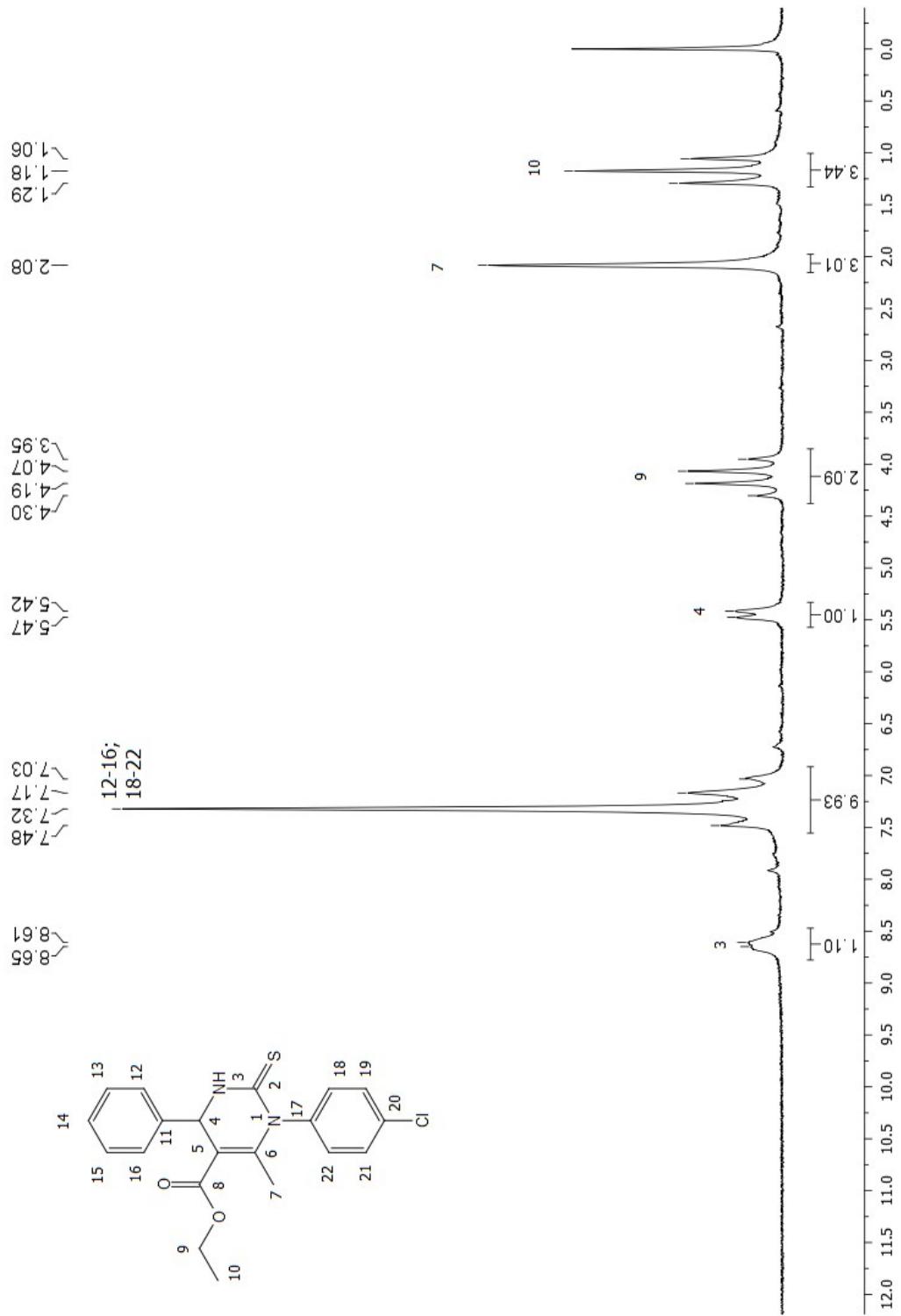


Figure S7. ^1H NMR spectrum (60 MHz, CDCl_3) of compound **19b**.

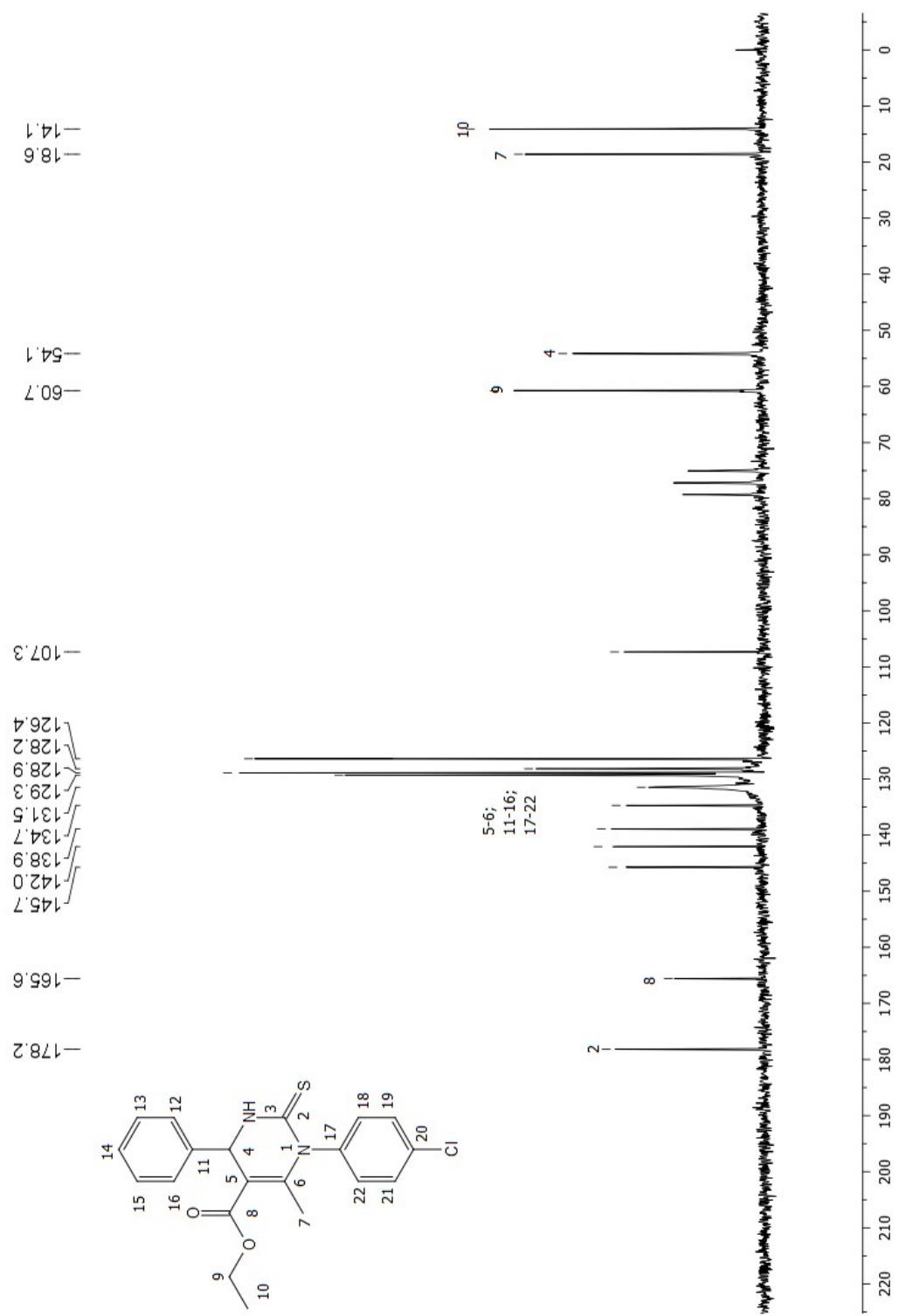


Figure S8. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19b.

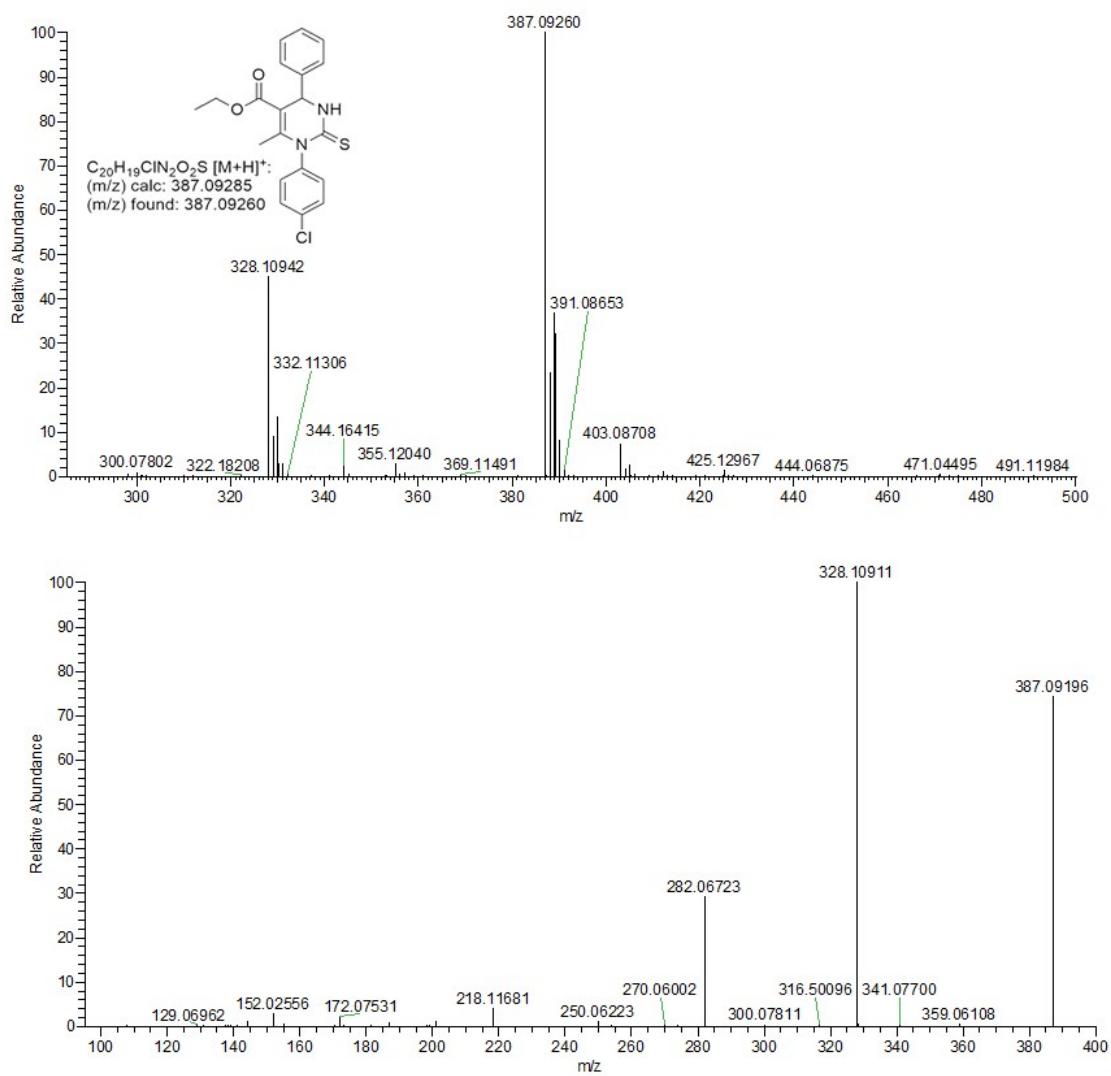


Figure S9. HRMS spectrum of compound **19b**.

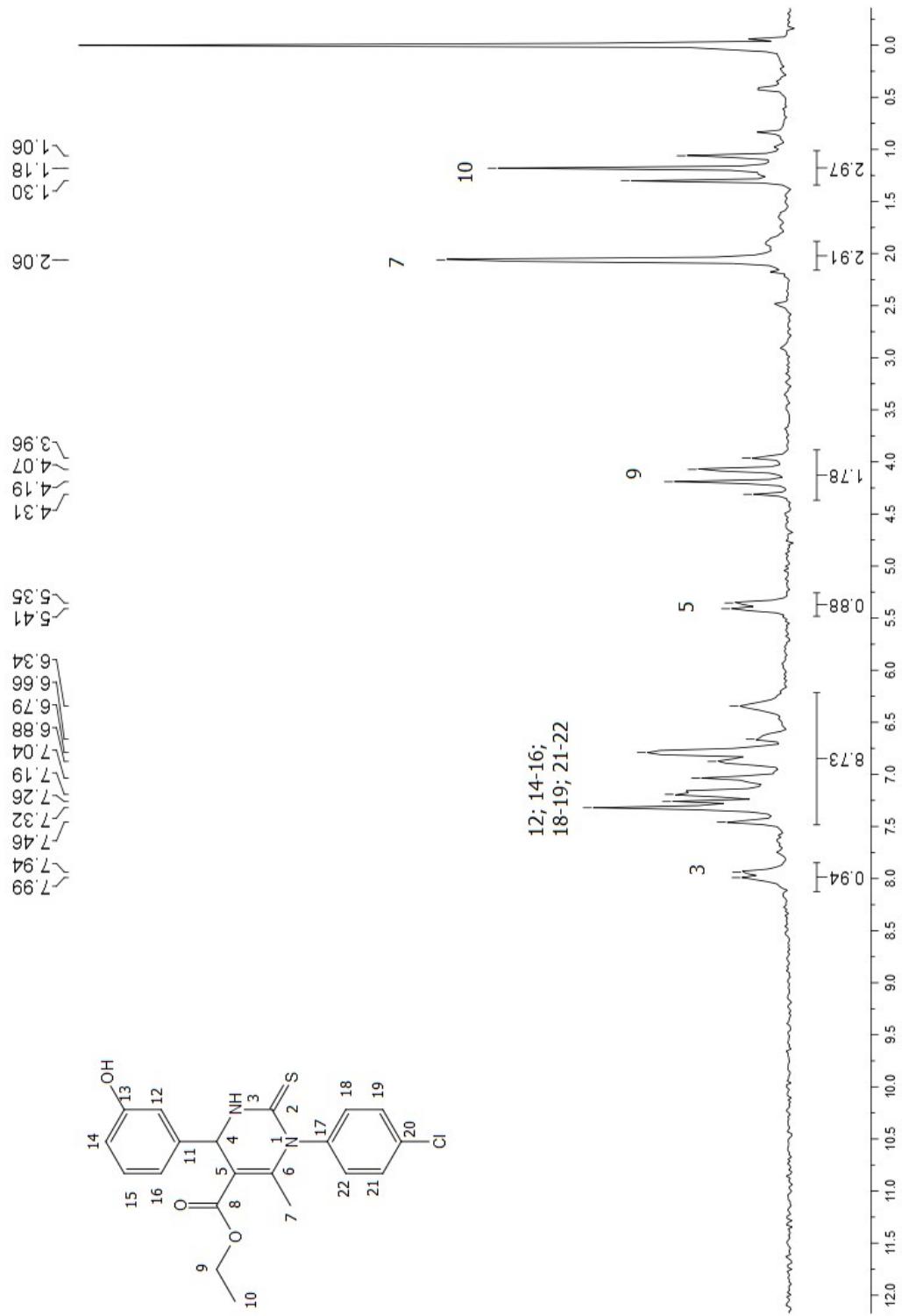


Figure S10. ^1H NMR spectrum (60 MHz, CDCl_3) of compound **20b**.

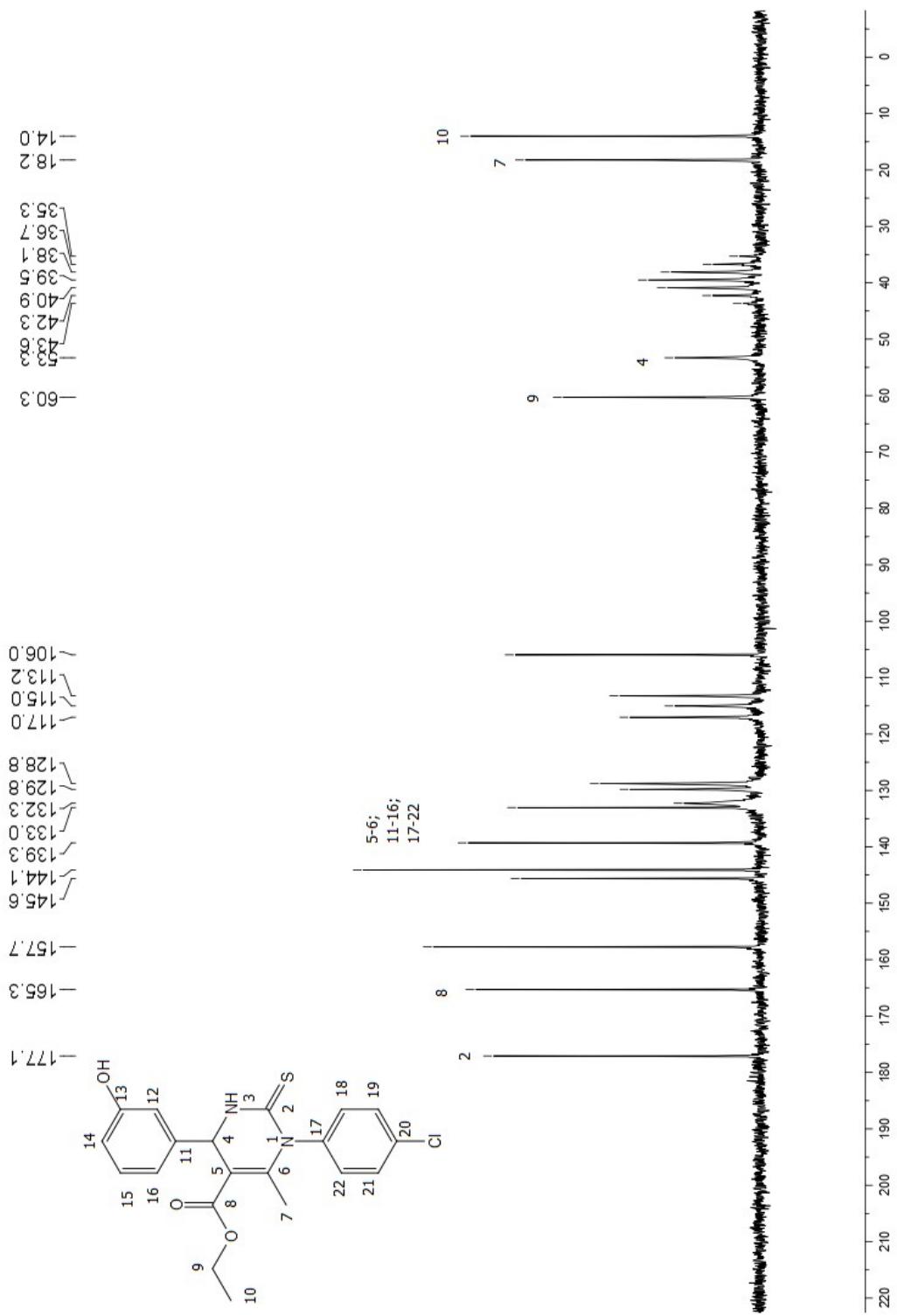


Figure S11. ^{13}C NMR spectrum (15 MHz, DMSO- d_6) of compound 20b.

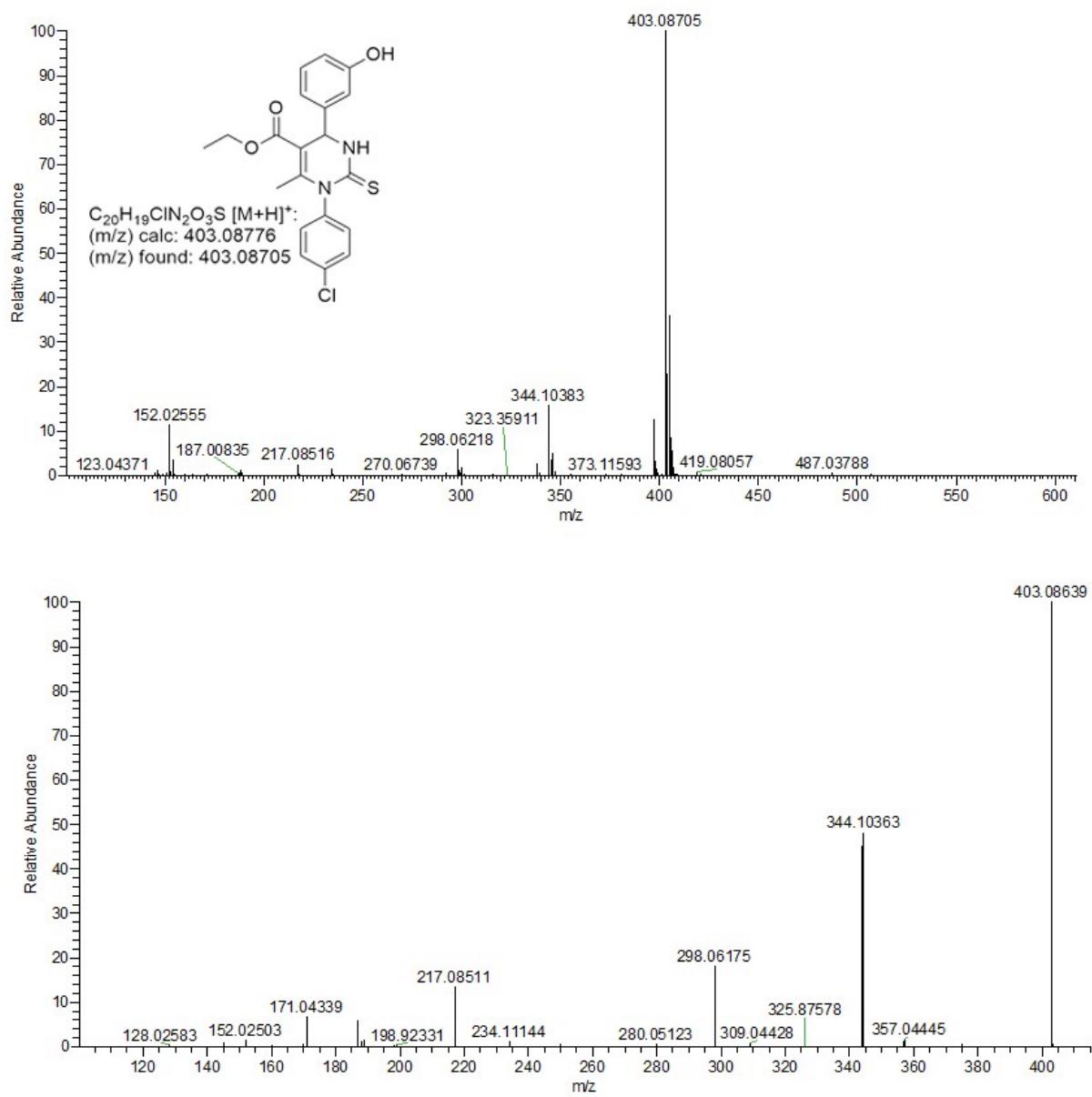


Figure S12. HRMS spectrum of compound **20b**.

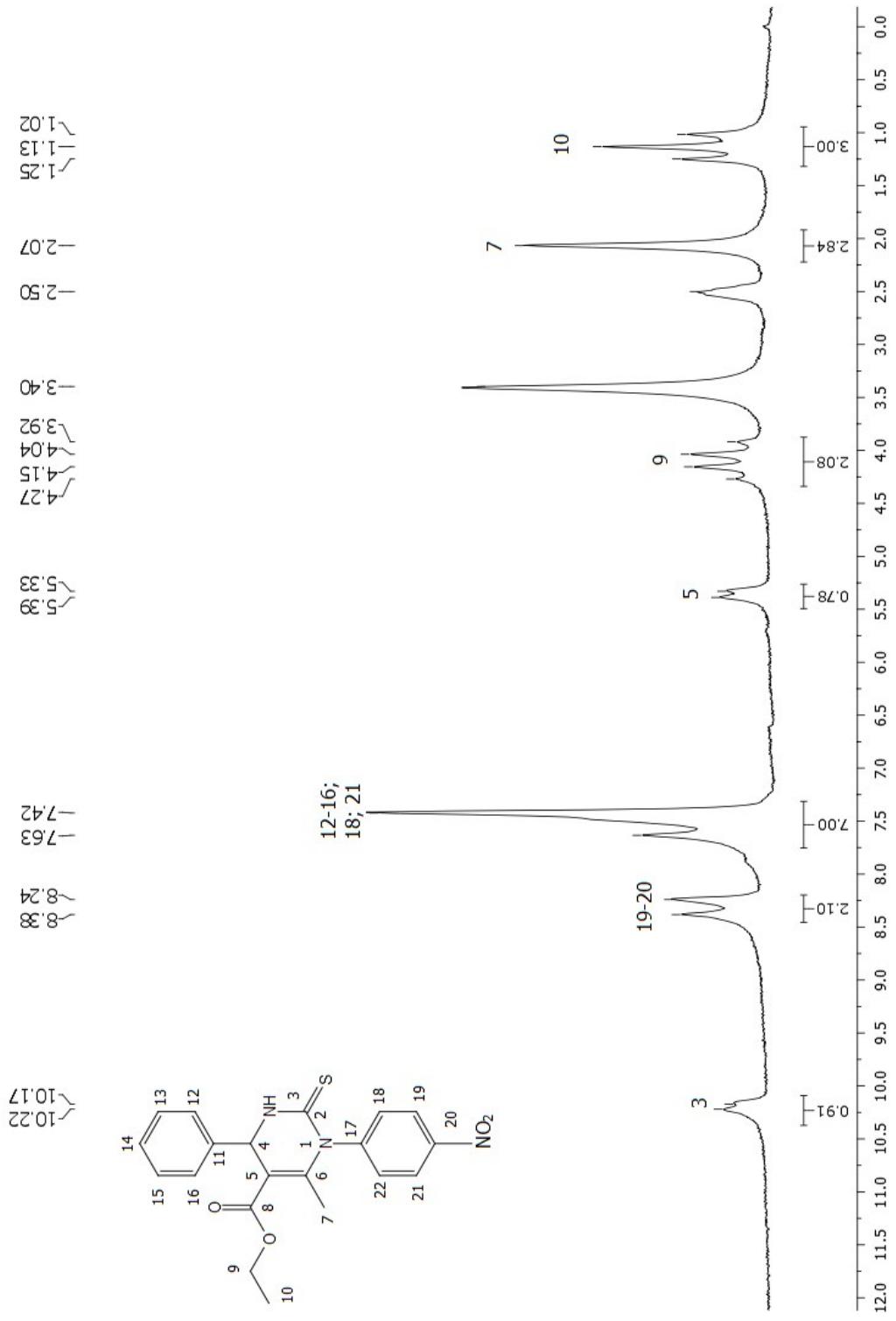


Figure S13. ^1H NMR spectrum (60 MHz, DMSO- d_6) of compound 19e.

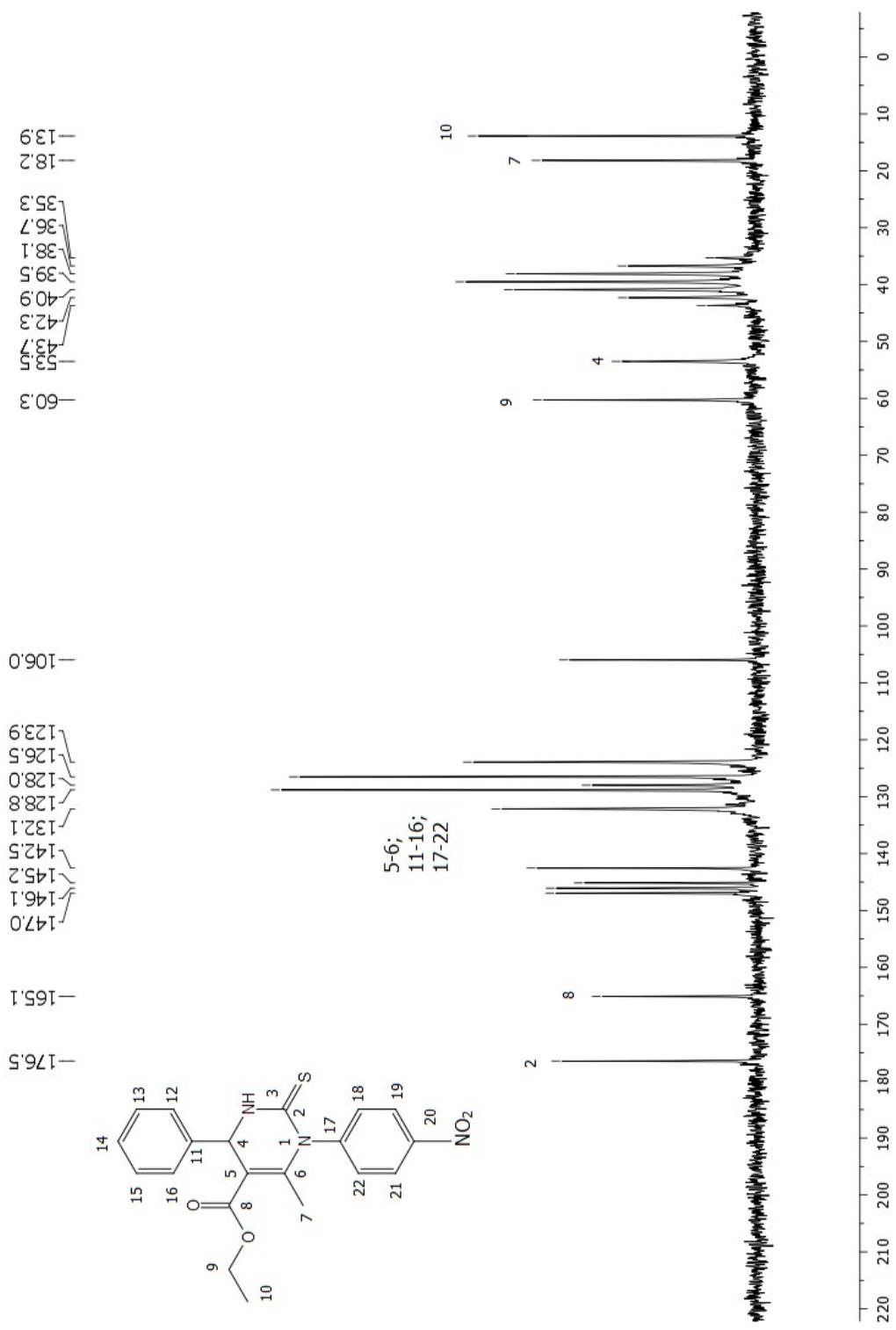


Figure S14. ^{13}C NMR spectrum (15 MHz, DMSO- d_6) of compound 19e.

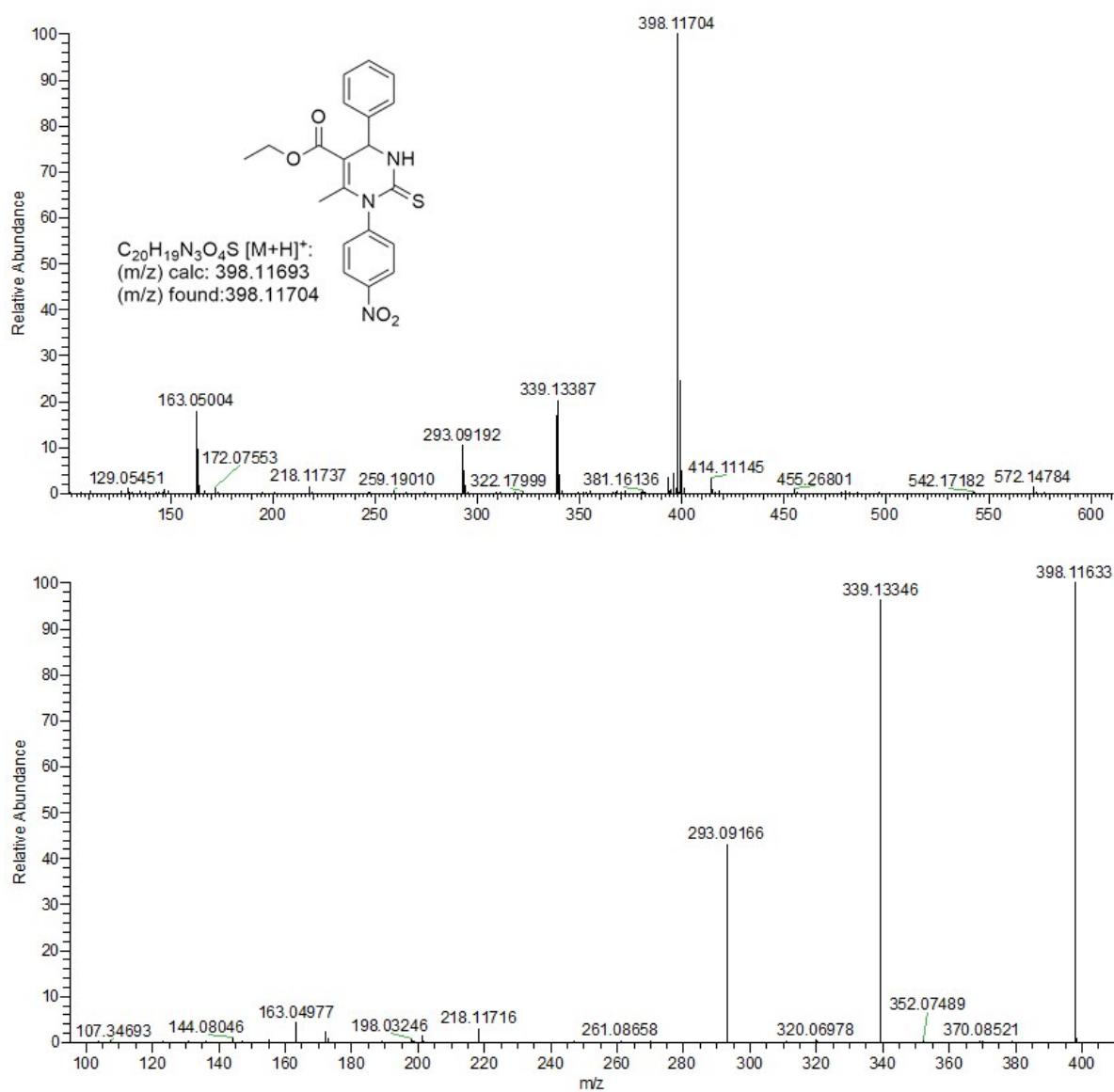


Figure S15. HRMS spectrum of compound **19e**.

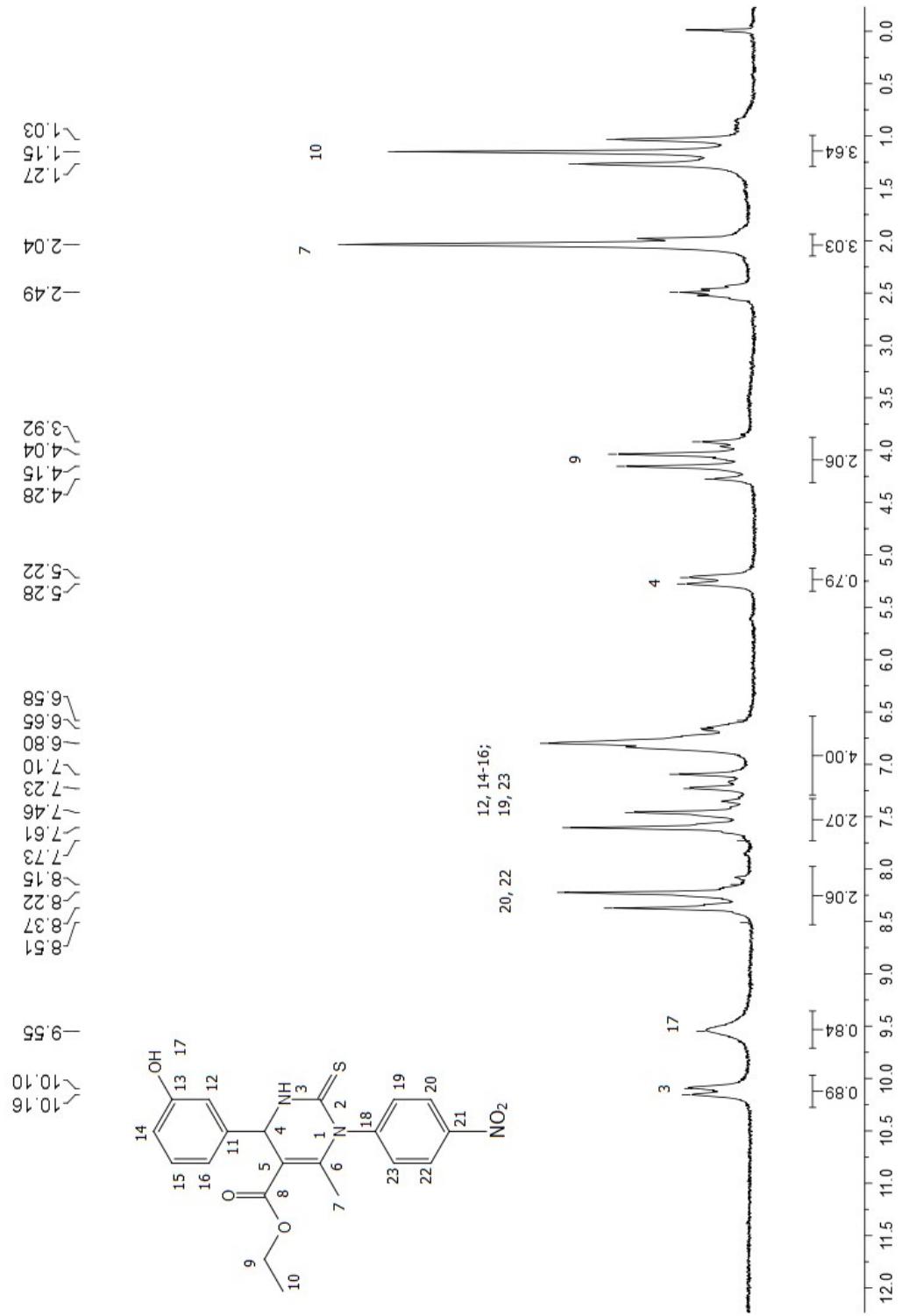


Figure S16. ^1H NMR spectrum (60 MHz, DMSO- d_6) of compound **20e**.

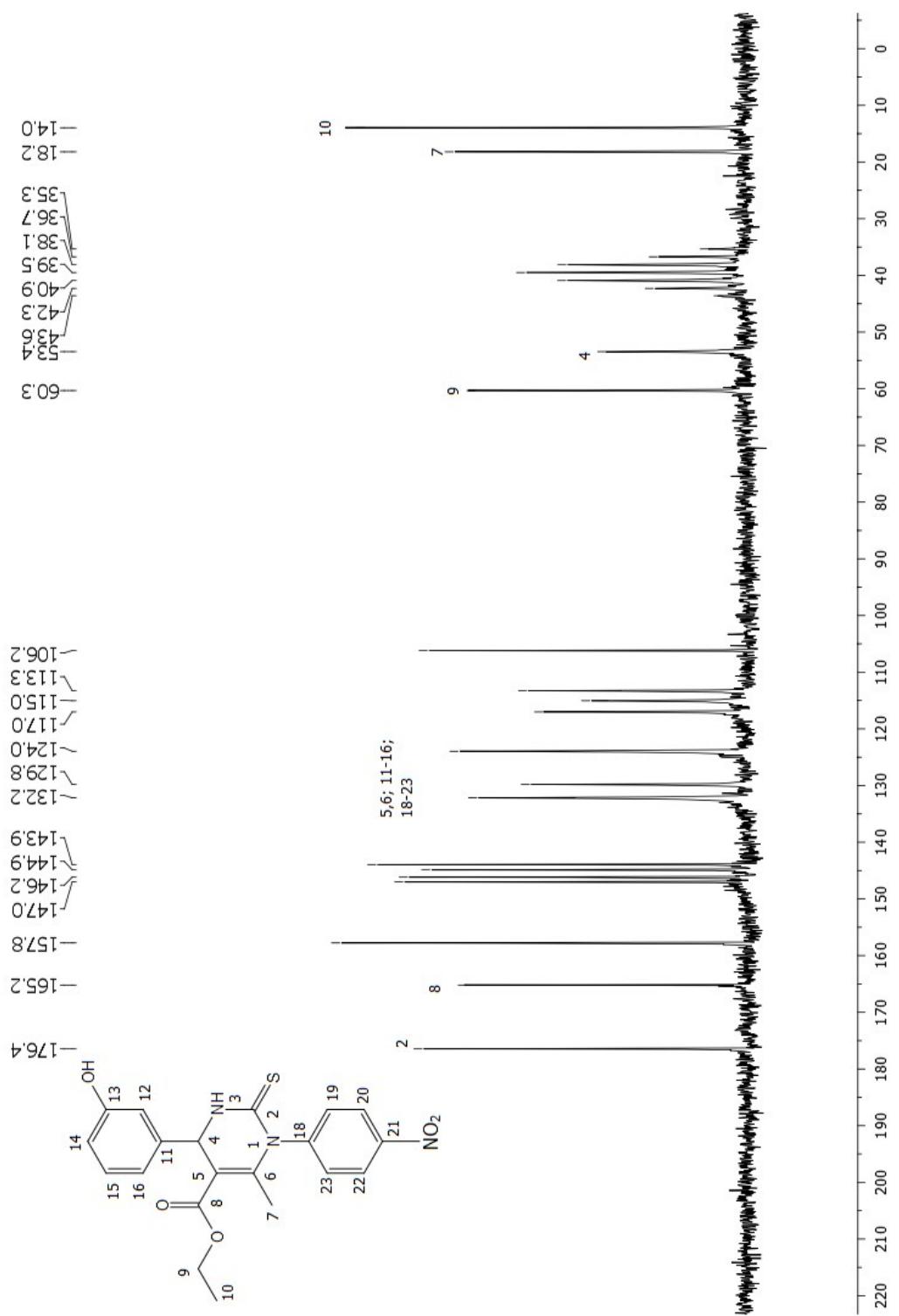


Figure S17. ^{13}C NMR spectrum (15 MHz, $\text{DMSO}-d_6$) of compound **20e**.

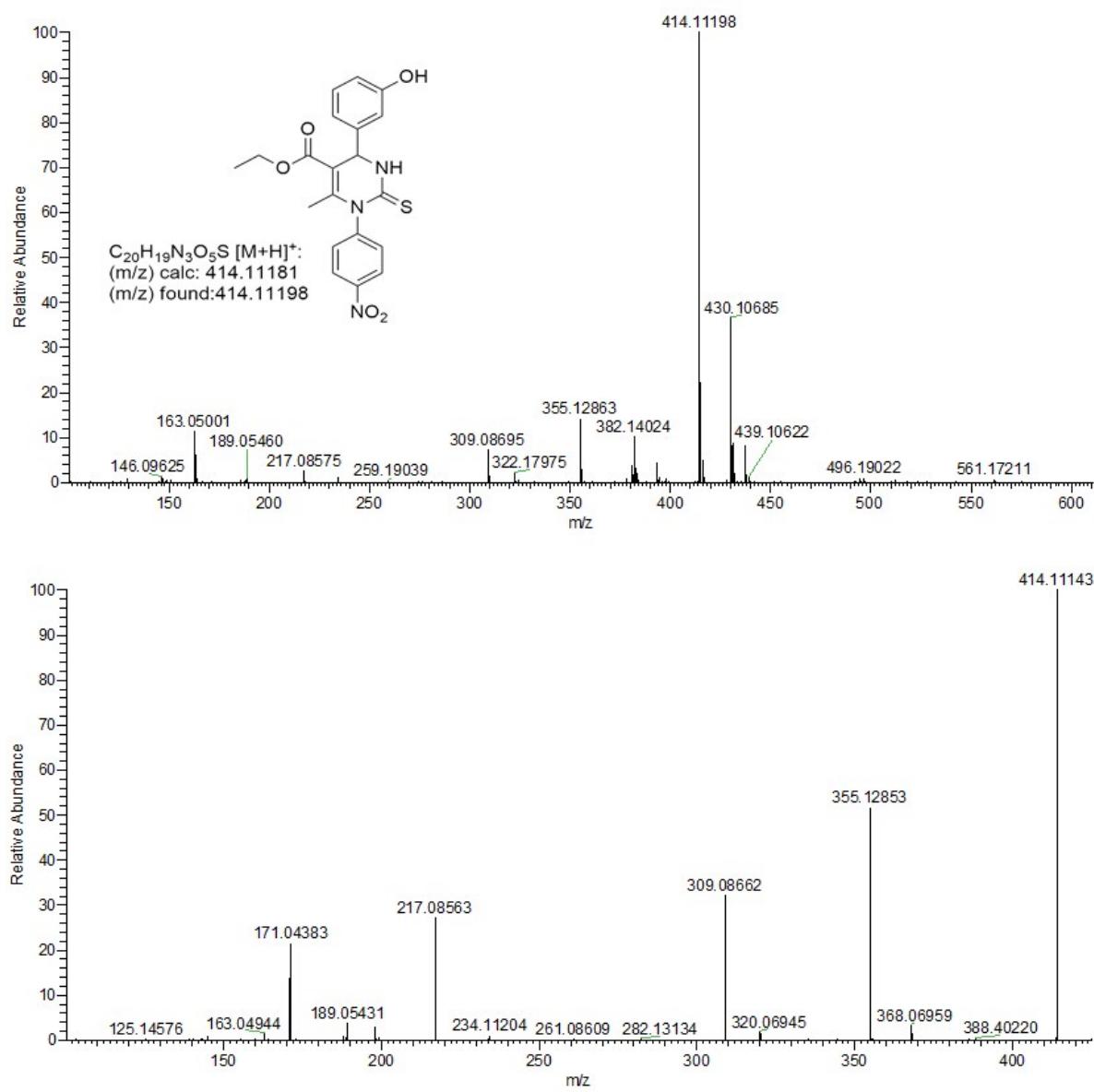


Figure S18. HRMS spectrum of compound **20e**.

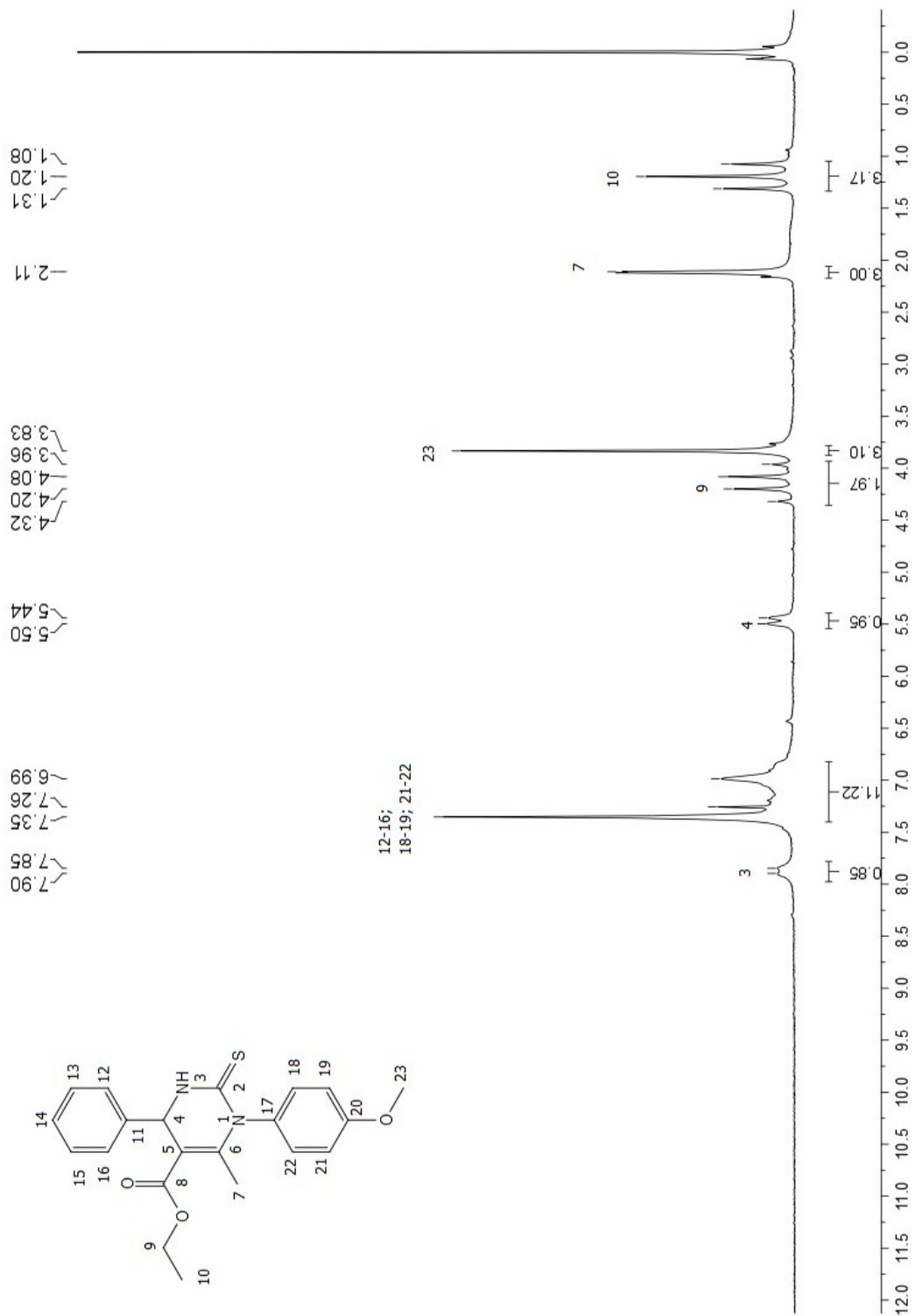


Figure S19. ¹H NMR spectrum (60 MHz, CDCl₃) of compound 19h.

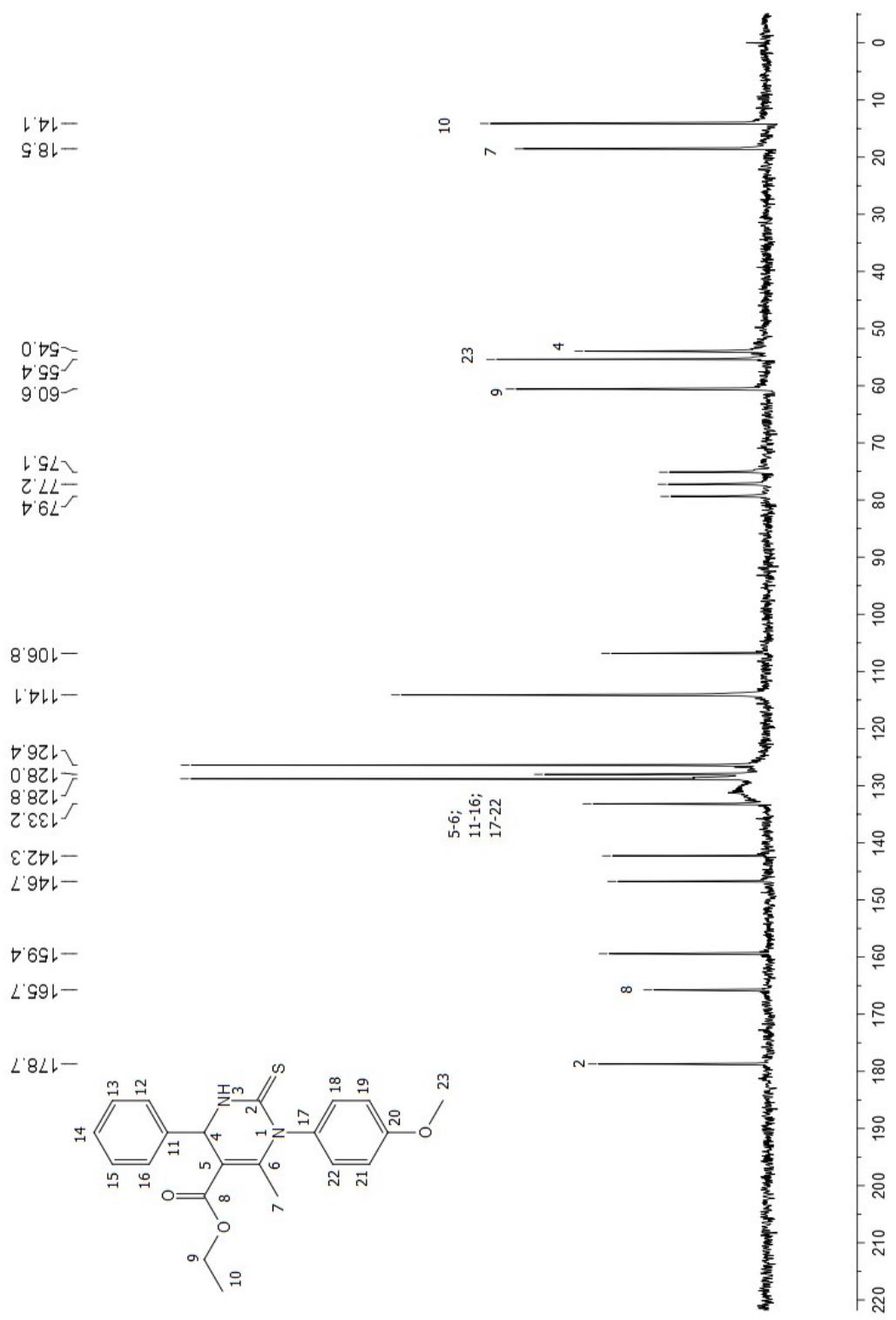


Figure S20. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19h.

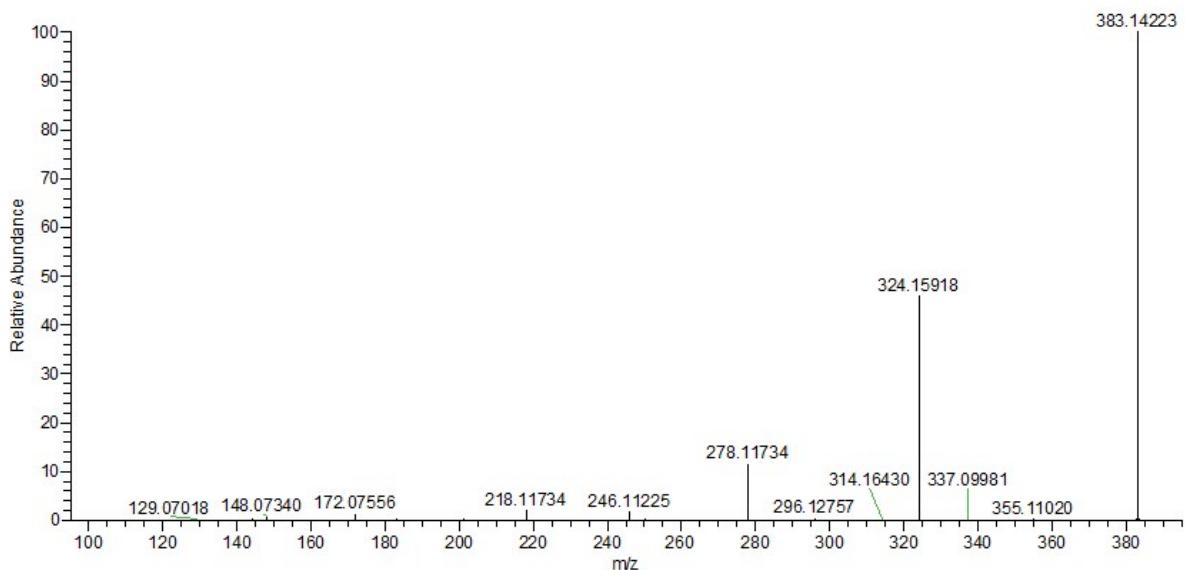
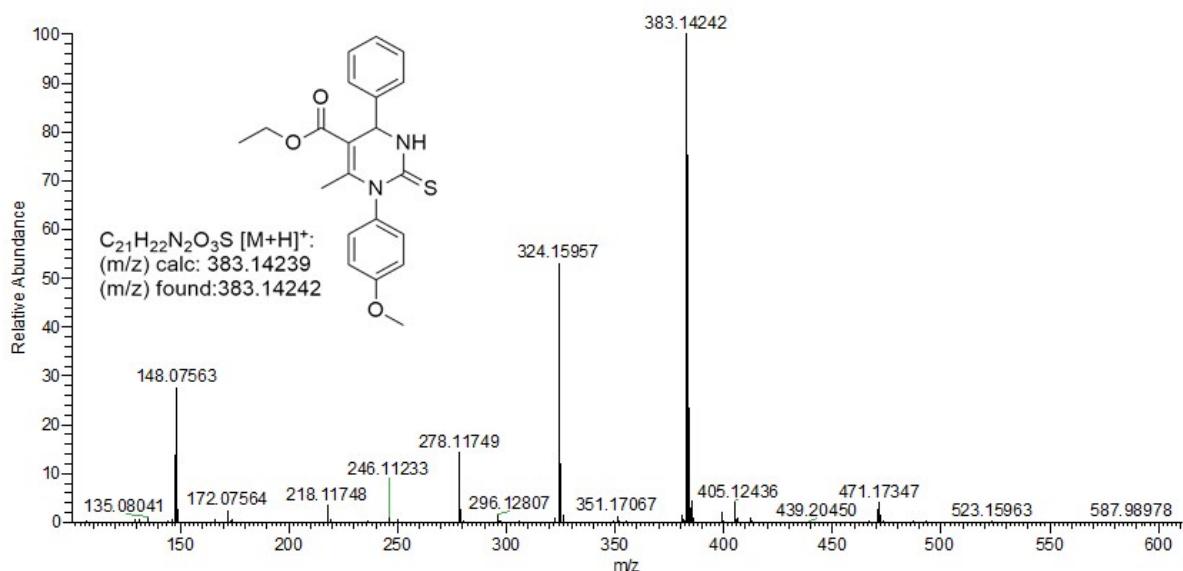


Figure S21. HRMS spectrum of compound **19h**.

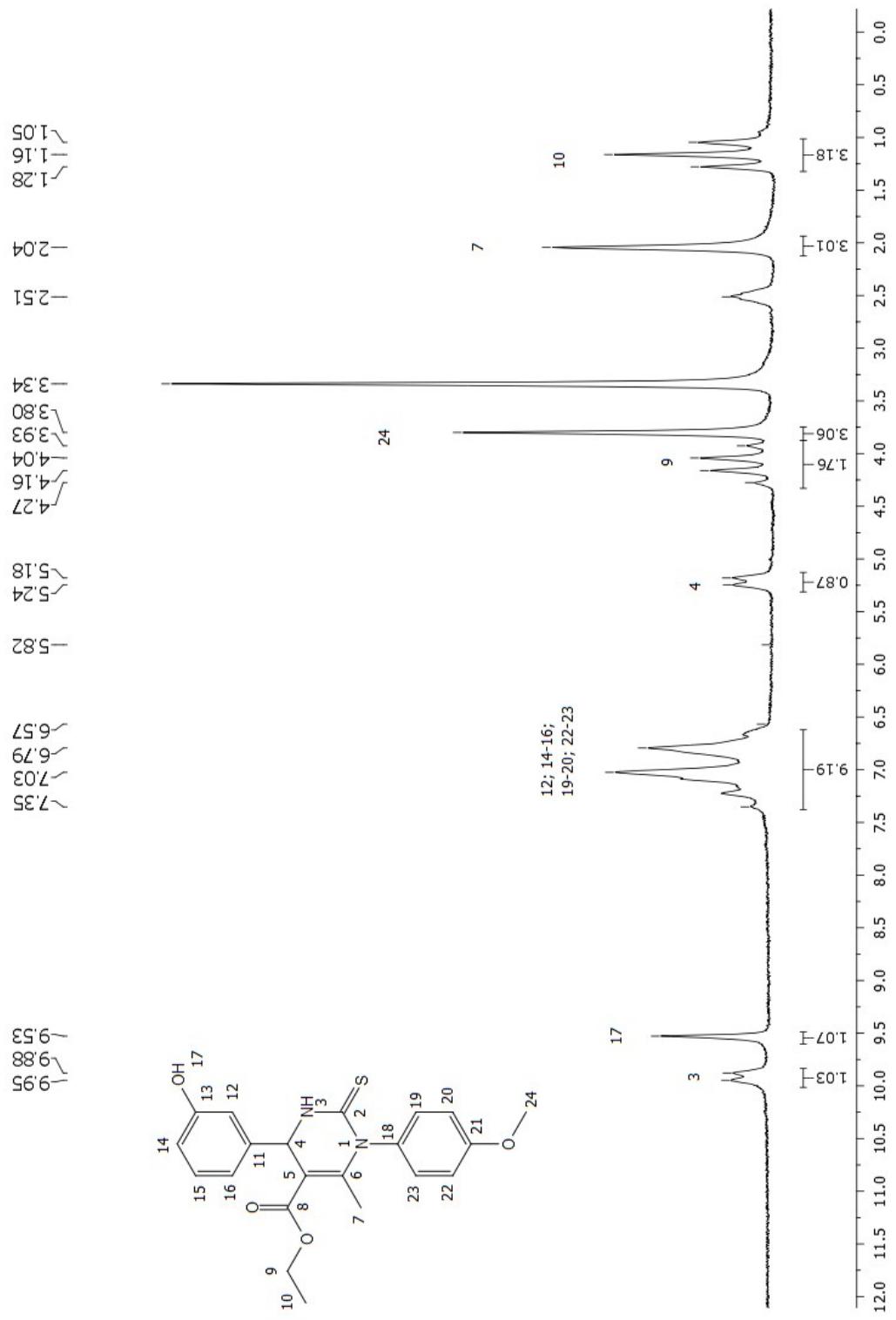


Figure S22. ^1H NMR spectrum (60 MHz, $\text{DMSO}-d_6$) of compound **20h**.

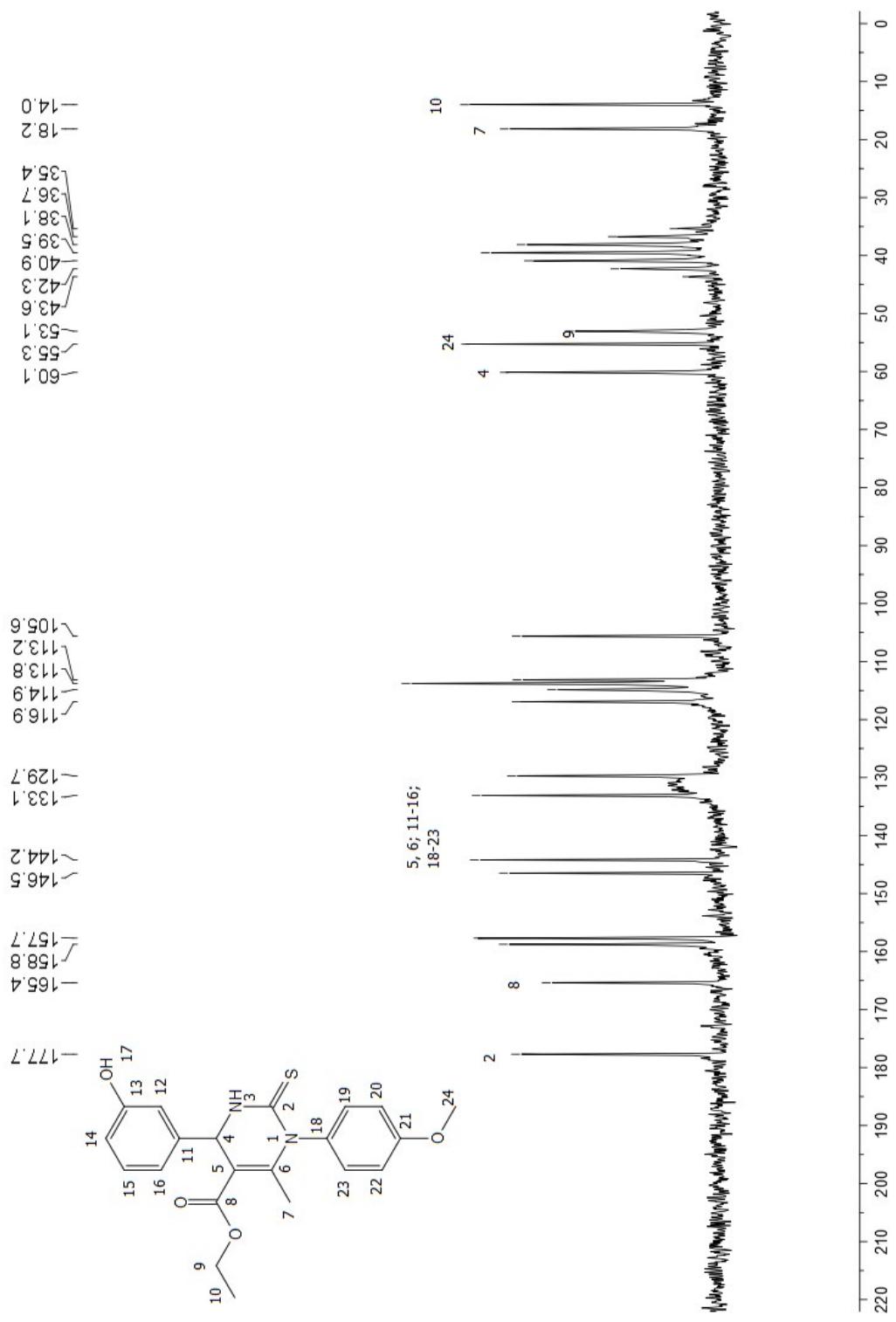


Figure S23. ^{13}C NMR spectrum (15 MHz, DMSO- d_6) of compound **20h**.

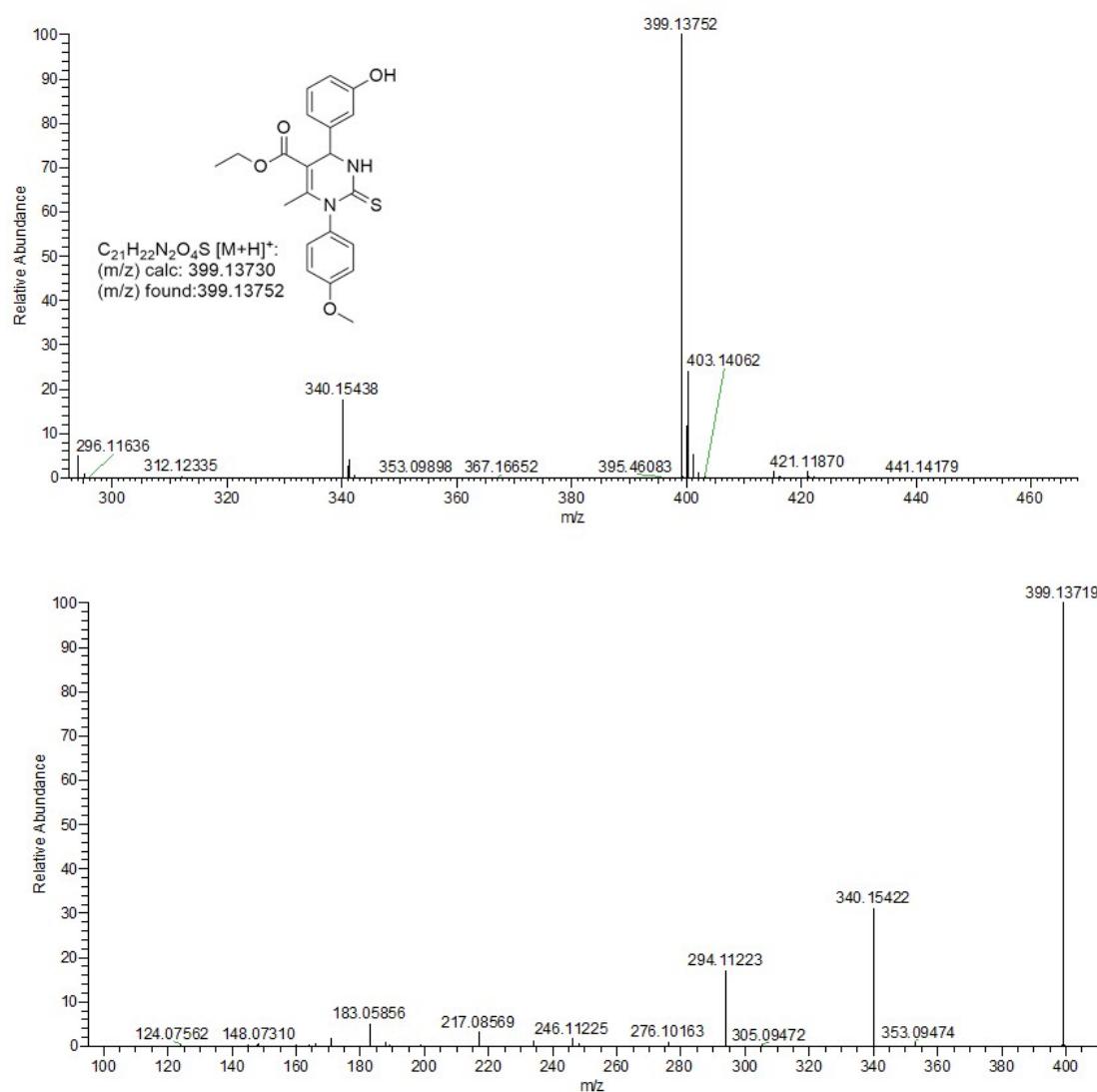


Figure S24. HRMS spectrum of compound **20h**.

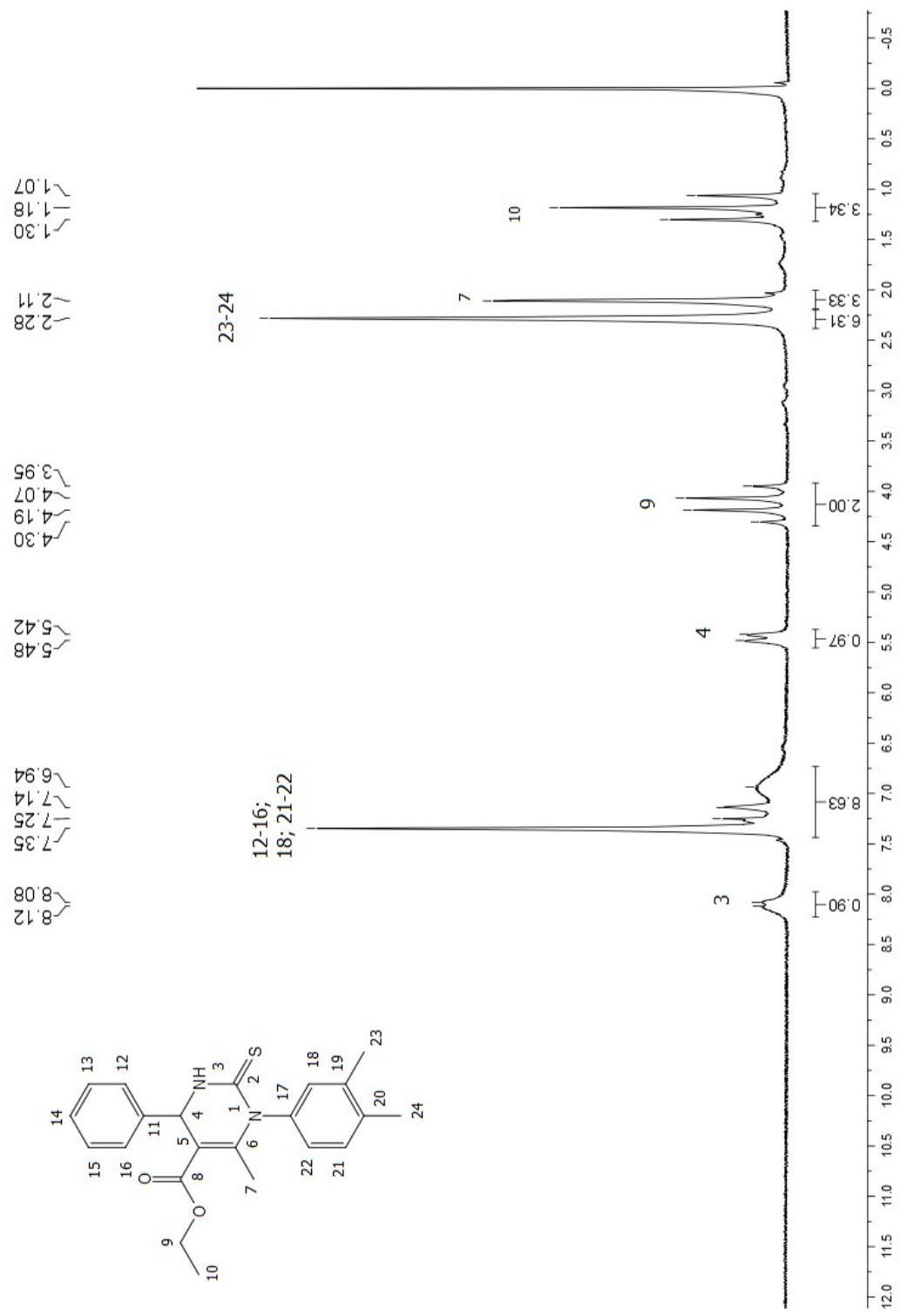


Figure S25. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 19k.

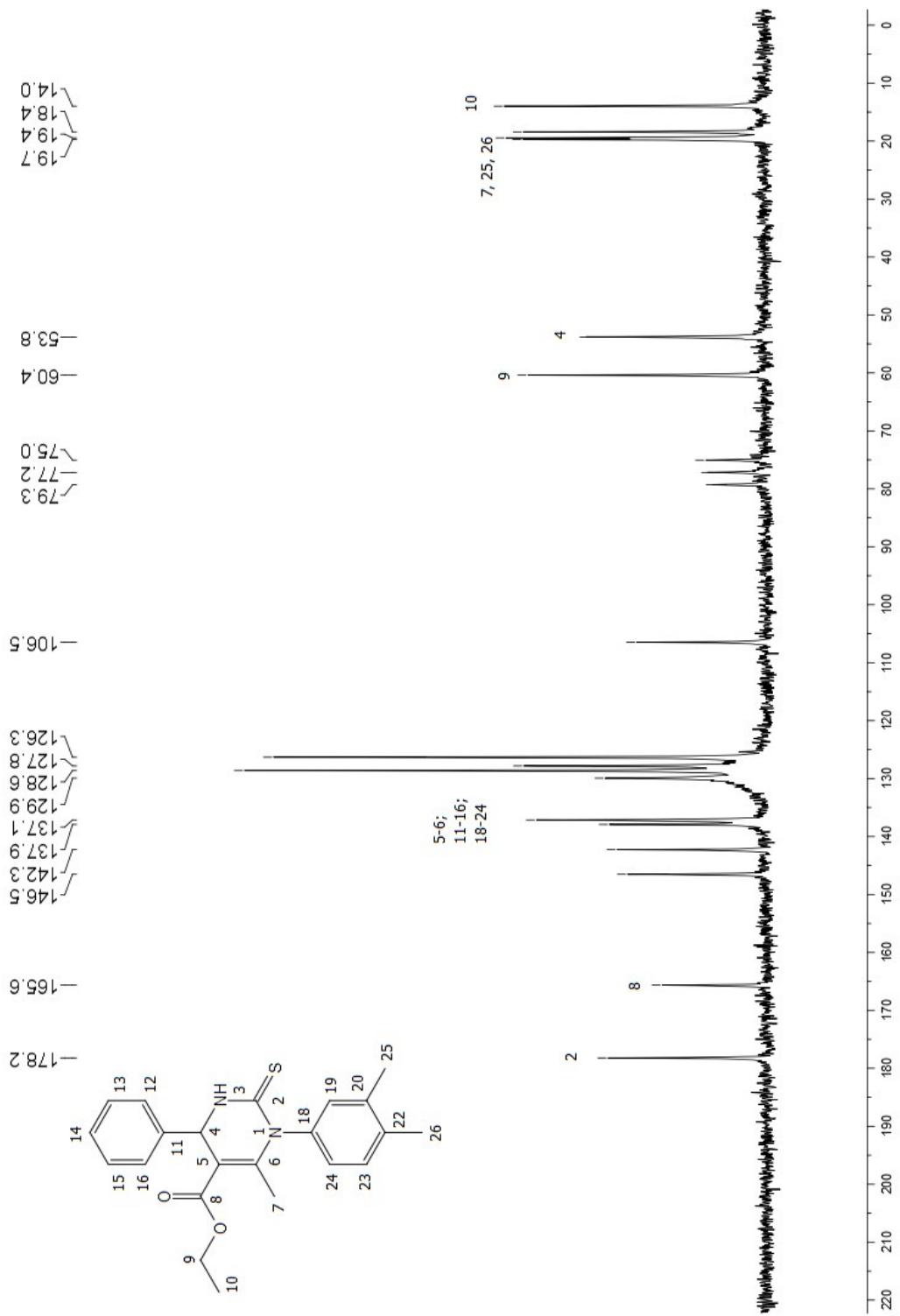


Figure S26. ^{13}C NMR spectrum (15 MHz, CDCl_3) of compound 19k.

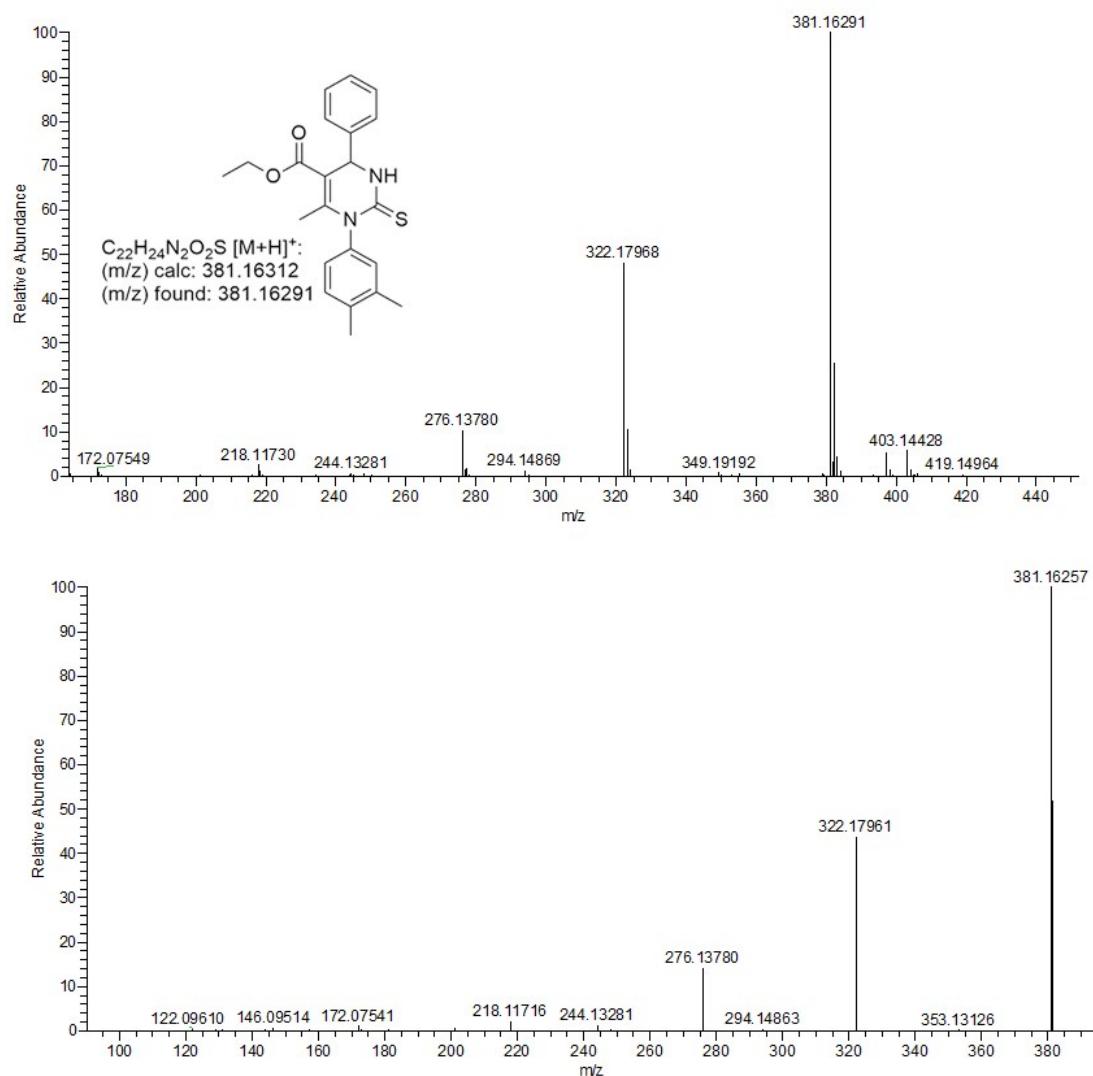


Figure S27. HRMS spectrum of compound **19k**.

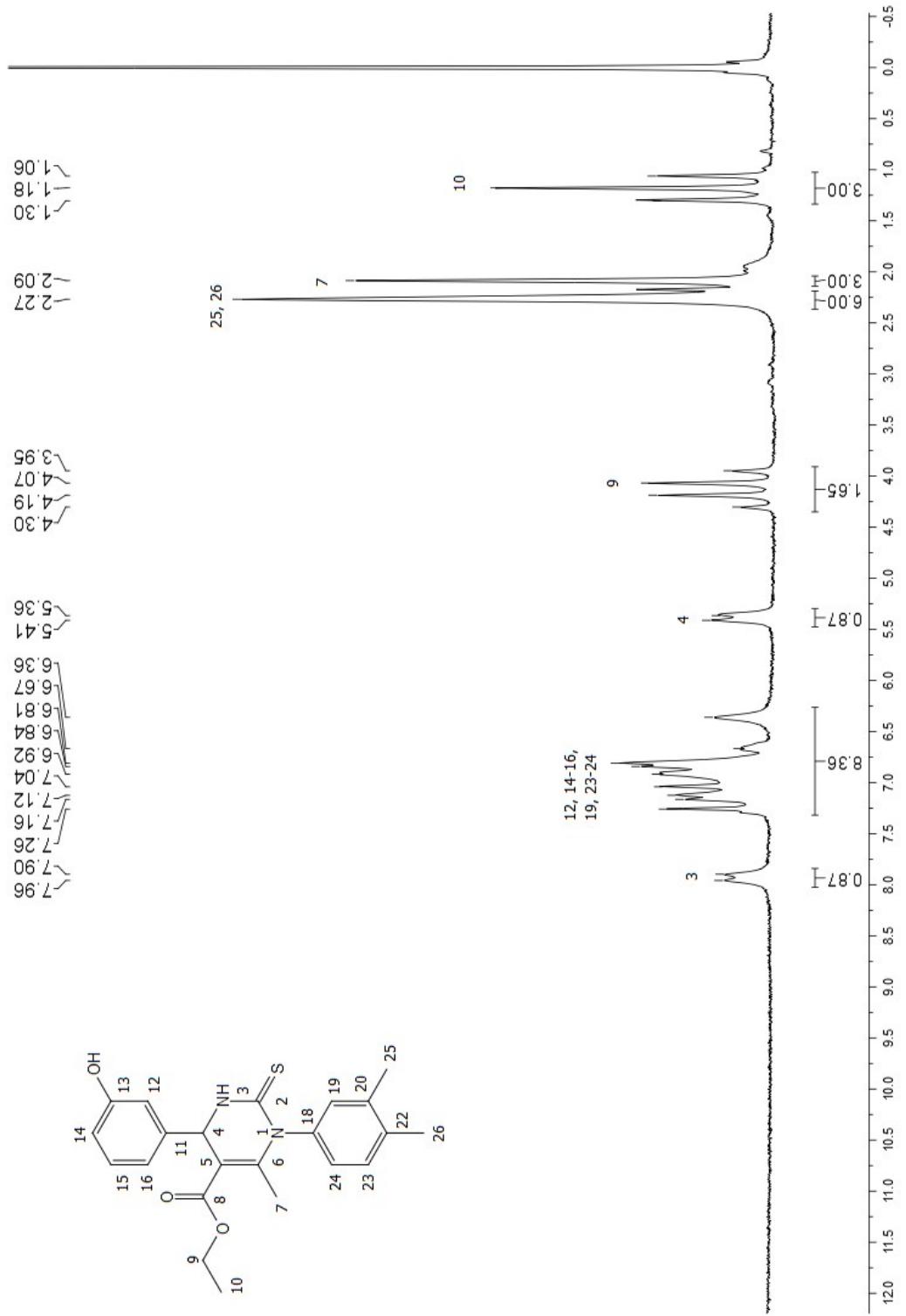


Figure S28. ^1H NMR spectrum (60 MHz, CDCl_3) of compound 20k.

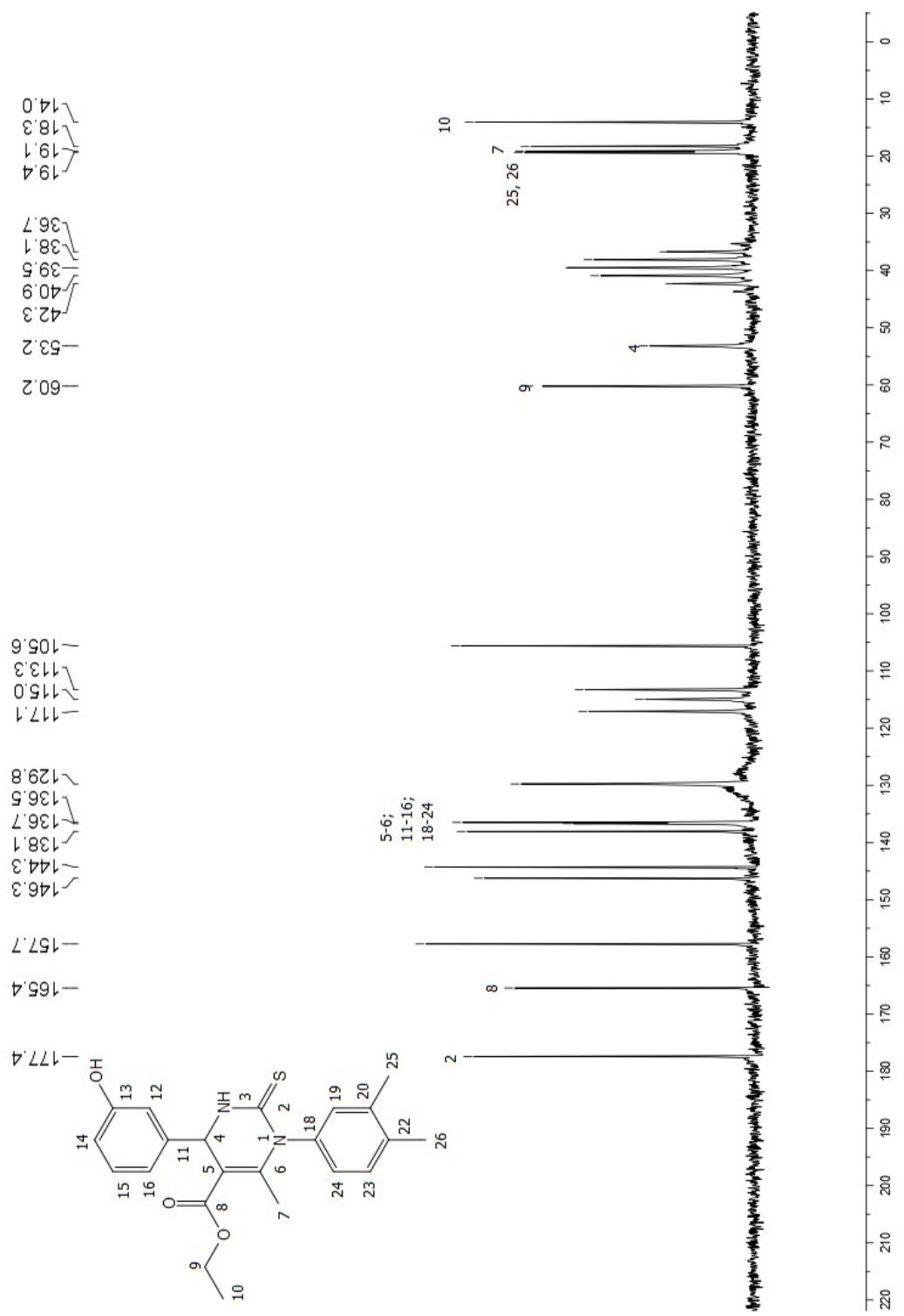


Figure S29. ^{13}C NMR spectrum (15 MHz, DMSO- d_6) of compound 20k.

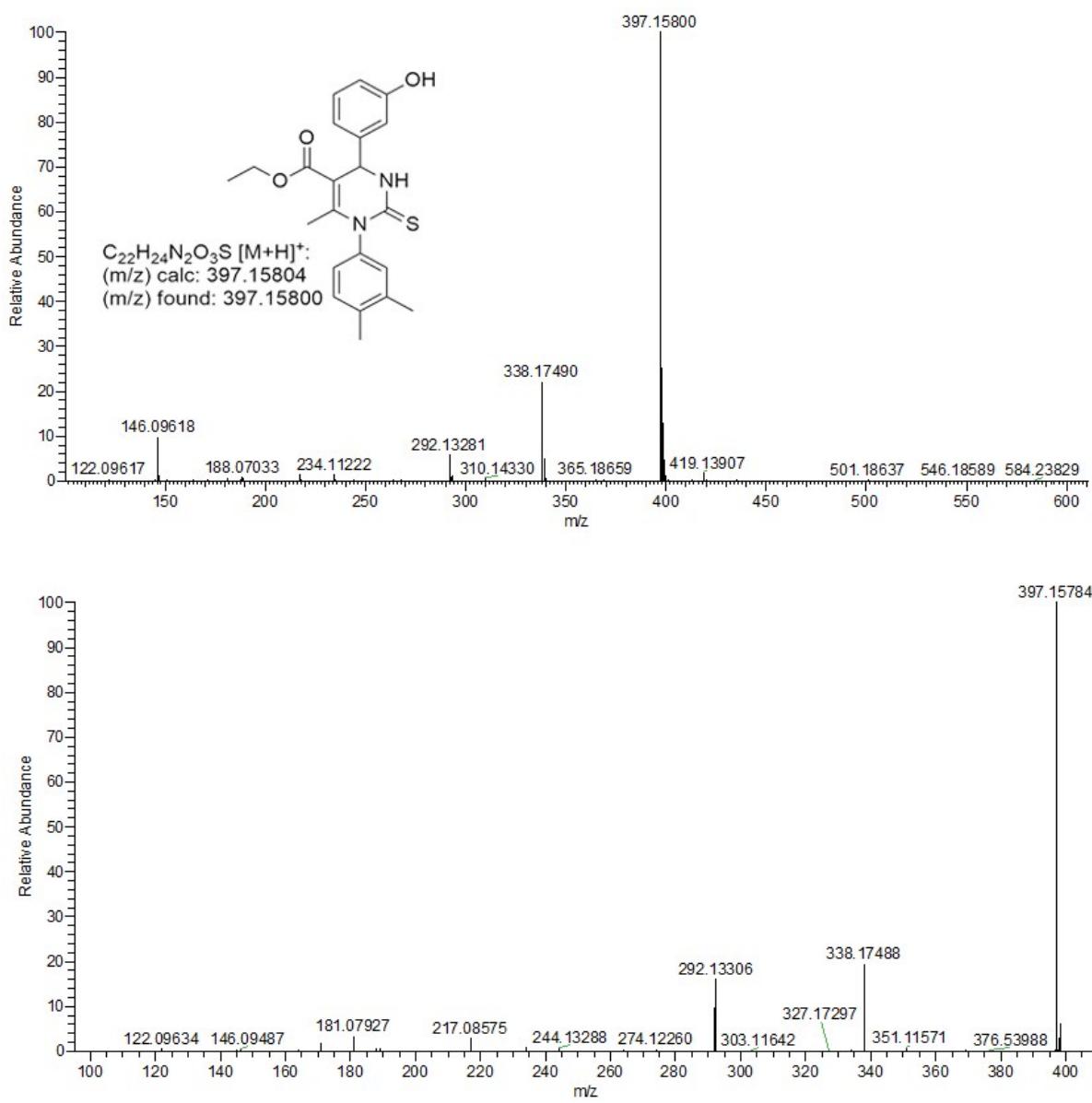


Figure S30. HRMS spectrum of compound **20k**.